



User Guide Version 6.2

Volume IV: Examples

$$\frac{\partial f_{el}}{\partial \Phi} - \frac{\partial f_e}{\partial \Phi}$$

“Resolution of partial differential equations is more about art than science”.

Apocryphal quotation from Numerical Recipes in Fortran

“ $2 + 2 = 4$ except for large values of 2”

Anonymous

“42”

Douglas Adams

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1 Introduction

The software MICRESS® (MICRostructure Evolution Simulation Software) is developed for time- and space-resolved numerical simulations of solidification, grain growth, recrystallisation or solid state transformations in metallic alloys. MICRESS® covers phase evolution, solutal and thermal diffusion and transformation strain in the solid state. It enables the calculation of microstructure formation in time and space by solving the free boundary problem of moving phase boundaries.

The microstructure evolution is governed essentially by thermodynamic equilibria, diffusion and curvature. In case of multicomponent alloys, the required thermodynamic data can either be provided to MICRESS® in the form of locally linearized phase diagrams, or by direct coupling to thermodynamic data sets via a special TQ interface, developed in collaboration with Thermo-Calc™ AB, Stockholm.

MICRESS® is based on the multi-phase-field method which defines a phase-field parameter for each phase involved. The phase-field parameter describes the fraction of each phase as a continuous function of space and time. Each single grain is mapped to a distinct phase-field parameter and is treated as an individual phase. A set of coupled partial differential equations is formed which describes the evolution of the phase-field parameter, together with concentration, temperature, stress and flow fields. The total set of equations is solved explicitly by the finite difference method on a cubic grid.

2D and 3D simulations are possible. The size of the simulation domain, the number of grains, phases and components is restricted mainly by the available memory size and the CPU speed.

Suggestions for improvements of the manual or comments on the manual are highly welcome to documentation@micress.de.



MICRESS® handles:

- 1-, 2- and 3-dimensional calculation domains
- arbitrary number of components, phases and grains
- solid-solid and solid-liquid interaction
- anisotropy of grain boundaries, mobility and energy

MICRESS® supports:

- coupling to thermodynamic database (via the TQ-interface of Thermo-Calc™)

In the present **MICRESS® User Guide Part IV: “MICRESS Examples”** you will find:

- an overview of available MICRESS® examples
- a short description of the different examples, their scope and the respective simulation conditions/parameters
- some visualized results for each example

Major scope of this manual is to provide a quick overview over the different examples and different MICRESS features used to run them without the need of visualizing the results with DP_MICRESS or stepping deeper into the respective driving files.

A description of the phase-field phenomenology and theoretical background can be found in *MICRESS Vol. 0: MICRESS Phenomenology*. *MICRESS Vol. I: Installing MICRESS* provides information about the installation of the software and explains how to verify successful installation with the help of simple examples. *MICRESS Vol. II: Running MICRESS* offers an overview of the input file structure, as well as theoretical and practical information on metallurgical processes, numerical modelling using the phase-field model and troubleshooting when starting a simulation. It provides useful hints on how to build the input file according to the process to be simulated. *MICRESS Vol. III: MICRESS Post-processing* explains the possibilities for analysing MICRESS output results.



2 What's new?

This section will be regularly up-dated with new examples for new features of MICRESS once they have become established examples.

For Release 6.2, the “Gamma_Alpha” family of examples has been completely reworked. Although the former versions of this family’s examples (Gamma_Alpha_dri, Gamma_Alpha_TC_dri, Gamma_Alpha_NPLE_dri, Gamma_Alpha_PARA_dri) proved to be a good basis for MICRESS courses and for demonstrating the general input file structures, the choice of parameters was quite extreme and thus not optimal for starting own research in the field of gamma-alpha transformations.

Consequently, the fundamental changes chosen were to strongly increase the alloying level in order to increase solutal control and to implement the nple (**n**o **p**artitioning – **l**ocal **e**quilibrium) redistribution model as default. To obtain meaningful results at a high computational performance (which is important for hands-on courses) the thermal boundary conditions further have been changed to isothermal while keeping the initial microstructure and the basic design of the nucleation types unchanged. The new members of the “Gamma_Alpha” family now are Gamma_Alpha_dri, Gamma_Alpha_TO_dri, Gamma_Alpha_PARA_dri, and Gamma_Alpha_PARATO_dri.

A completely new example, CMSX4_dri has been added to the collection in order to demonstrate simulation of the directional solidification of a complex 10-component alloy in the isothermal cross-section including a grain boundary. Main features are the formation of primary dendrites and the interdendritic precipitation of γ' phase. Several “advanced” features of MICRESS 6.2 are used in this example.

Examples for flow solver usage have been provided and are described in the sections “Dendrites” and “Flow”. “Dendrites” consists of two examples, one without and one with melt flow, simulating growth of a three dimensional equiaxed dendrite in AISi7 with concentration coupling.

The “Flow” examples simulate fluid flow for a static phase field. The “Flow_Cylinder” examples show how the flow pattern around a cylinder differs for different Reynolds numbers. The “Flow_Permeability” example shows how to read in a structure and simulate fluid flow to determine its permeability.





3 Examples Overview

MICRESS® examples are located in the MICRESS® installation directory or can be downloaded from the web (www.micress.de). They do not cover the entire range of applications of the software, but treat some typical cases and can be used as starting points for other purposes. They also do not exploit the full complexity of the MICRESS software, which has already successfully been applied to technical alloy systems with more than 14 different thermodynamic phases, but rather demonstrate its basic features on the basis of simple examples.

The following tables give an overview of the features covered in the examples. There are basically two examples categories. The first, table 1, comprises “solid state transformation” examples, whereas the second, table 2, is dedicated to “solidification” examples.

Example		Gamma_Alpha_dri	Gamma_Alpha_PARA_dri	Gamma_Alpha_TQ_dri	Gamma_Alpha_PARATQ_dri	GammaAlpha_Stress_dri	GammaAlphaCementite_TQ_dri	GammaAlphaCementite_LinTQ_dri	GammaAlphaPearlite_TQ_dri	Grain_Growth_dri	Grain_Growth_Pinning_Pres_dri	Grain_Growth_Solute_Drag_dri	Grain_Growth_Solute_Drag_dG_dri	Grain_Growth_Profiles_dri	Grain_Growth_3D_dri	Stress_dri	FeMn_m64_intf_dri	ReX_deterministic_dri	ReX_local_Humpreys_dri	ReX_local_recovery_dri	ReX_mean_dislocation_dri	ReX_random_dri
number		01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21
alloy		Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn													



transformation		solid state	solid state	solid state	solid state	solid state	solid state	solid state	solid state	grain growth	grain growth	grain growth	grain growth	grain growth	grain growth	solid state	recrystallisation	recrystallisation	recrystallisation	recrystallisation	recrystallisation	recrystallisation
concentration coupling		X	X	X	X	X	X	X	X							X	X					
temperature coupling																						
only phase field										X	X	X	X	X	X			X	X	X	X	X
stress field						X										X						
fluid flow																						
recrystallisation																	X	X	X	X	X	X
dimension	1D					X																
	2D	X	X	X	X		X	X	X	X	X	X	X	X		X	X	X	X	X	X	X
	3D															X						
time step	automatic	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X
	manual																					
microstructure	directional																					
	equiaxed	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X
initial microstructure	deterministic	X	X	X	X												X	X	X		X	
	random					X	X	X	X					X		X				X		X
	from file									X	X	X	X									
	voronoi	X	X	X	X	X	X	X	X					X		X	X	X	X	X	X	X
	restart																					
nucleation model	nucleation	X	X	X	X	X	X	X	X										X		X	X
	seed density																					
	seed undercooling	X	X	X	X	X	X	X	X										X		X	X
	recrystallisation																					



thermodynamic databases	thermo-dynamic coupling			X	X		X	X	X							X							
	diffusion data from database			X	X		X	X	X														
anisotropy model	cubic						X	X	X					X		X		X	X	X	X	X	X
	hexagonal																						
	faceted																						
	antifaceted																						
	misorientation																X	X	X	X	X	X	X
boundary conditions	1d far field																						
	1d field for temperature coupling																						
	moving frame																						
	latent heat																						
phase interaction modes	solute drag										X	X											
	particle pinning									X													
	redistribution control	X	X	X	X																		

Table 1 Overview of the “solid state transformation” features covered in the MICRESS examples



Example		AlCu_dri		AlCu_Equiaxed_dri		AlCu_Temp1d_dri		AlSi_trapping_dri		AlSi_trapping_ATC_dri		AlSi_trapping_ATC_mob_corr_dri		P_Peak_1D_dri		P_Peak_2D_dri		Delta_Gamma_dri		TQ_Eutectic_dri		TQ_Ripening_dri		CMSX4_dri		Temperature_dri		Dendrite_AISI_3D_dri		Dendrite_AISI_3D_flow_dri		Flow_Cylinder_Laminar_dri		Flow_Cylinder_Karman_dri		Flow_Permeability_dri					
number		22		23		24		25		26		27		28		29		30		31		32		33		34		35		36		37		38		39					
alloy		Al-Cu		Al-Cu		Al-Cu		Al-Si		Al-Si		Al-Si		Fe-C-Mn-P-Si		Fe-C-Mn-P-Si		Fe-C-Mn		Al-Ag		Al-Ag		CMSX4				AISI7		AISI7											
transformation		solidification		solidification		solidification		solid-liquid		solid-liquid		solid-liquid		peritectic		peritectic		peritectic		eutectic		solid-liquid		solidification		solidification		solidification		solidification											
concentration coupling		X		X		X		X		X		X		X		X		X		X		X		X			X		X												
temperature coupling																									X																
only phase field																															X		X		X						
stress field																																									
fluid flow																													X		X		X		X						
recrystallisation																																									
dimension	1D					X		X		X		X																													
	2D	X		X		X								X		X		X		X		X		X		X					X		X								
	3D																										X		X						X						
time step	automatic	X		X		X		X		X		X		X		X		X		X		X		X		X		X		X					X						
	manual																														X		X								
microstructure	directional	X																X						X																	
	equiaxed			X		X								X					X		X			X		X		X		X											
microstructure	deterministic					X		X		X		X		X		X		X					X		X						X		X								
	random																		X		X																				

Table 2 Overview of the “solidification” features covered in the MICRESS examples



4 “Delta-Gamma”

4.1 Description

“Delta_Gamma_dri” is a 2D-simulation of the directional solidification of a ternary steel model alloy containing carbon and manganese. The simulation shows the solidification of a δ -phase dendrite and the subsequent peritectic reaction to the γ -phase. The simulation is performed as concentration-coupled and makes use of the 1d far field approximation and the moving frame option. It is coupled to Thermo-Calc™.

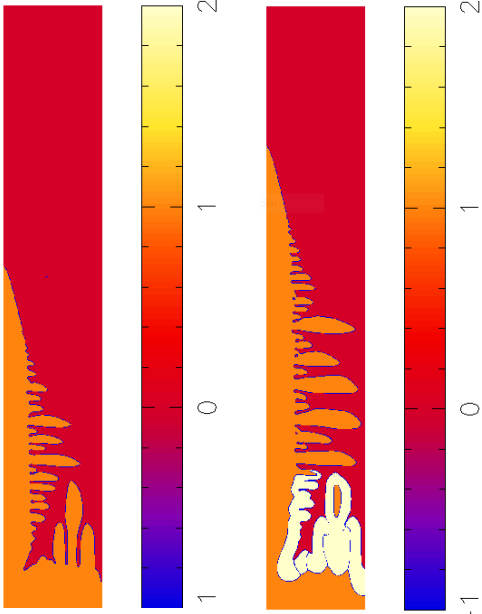
name dri file	Delta_Gamma.dri		
alloy system	Fe-C-Mn (Steel.Ges5)		
composition	98 at% Fe 1 at% C 1 at% Mn		
transition	solidification, peritectic transformation		

Figure 4.1. Example Delta_Gamma.phas: dendritic solidification at a time of 25 s (left) and peritectic reaction at a time of 32.5 s (right)



4.2 Simulation conditions

name dri file	Delta_Gamma.dri
dimension	2D
grid size	145x1500 cells
grid spacing	1 μm
interface thickness	4 cells
boundary conditions	East: symmetric West: symmetric bottom: insulated top: fixed
solid phases:	Two solid phases: δ phase, γ phase
grain input	<u>deterministic</u> placement of 1 grain of δ -phase (round $r = 0,0$; position $x = 0,5$, $z = 0,5$; stabilisation of the grain) <u>further nucleation</u> : γ -phase: seed position: interface; curvature undercooling; max. 5 seeds, $\Delta T = 1$ K, rotation angle -5° to 5° ; between 1765 K and 1700 K <u>temperature conditions</u> : $T_0 = 1786$ K; $G = 250$ K/cm; $dT/dt = -1$ K/s
output	<u>files</u> : restart, phases, average table fraction, interface, driving force, concentrations (C, Mn) <u>times</u> : -> fixed output at 0,01 s, 1,0 s and 2,5 s -> from 2,5 s to 35 s output every 2,5 s (linear step) -> from 35 s to 50 s output every 5,0s (linear step)
special features	-> concentration coupling -> 1d far field diffusion approximation (500 cells, distance from the front 200 μm) -> thermodynamic coupling (GES-file: Steel.GES5) -> moving frame (distance from the upper boundary 200 μm)

Table 3 Example Delta-Gamma: simulation conditions/parameters



4.3 Visualisation of the results

- Solidification sequence is presented by the .phas-output (-1: interface; 0: liquid; 1:

δ phase; 2: γ phase)

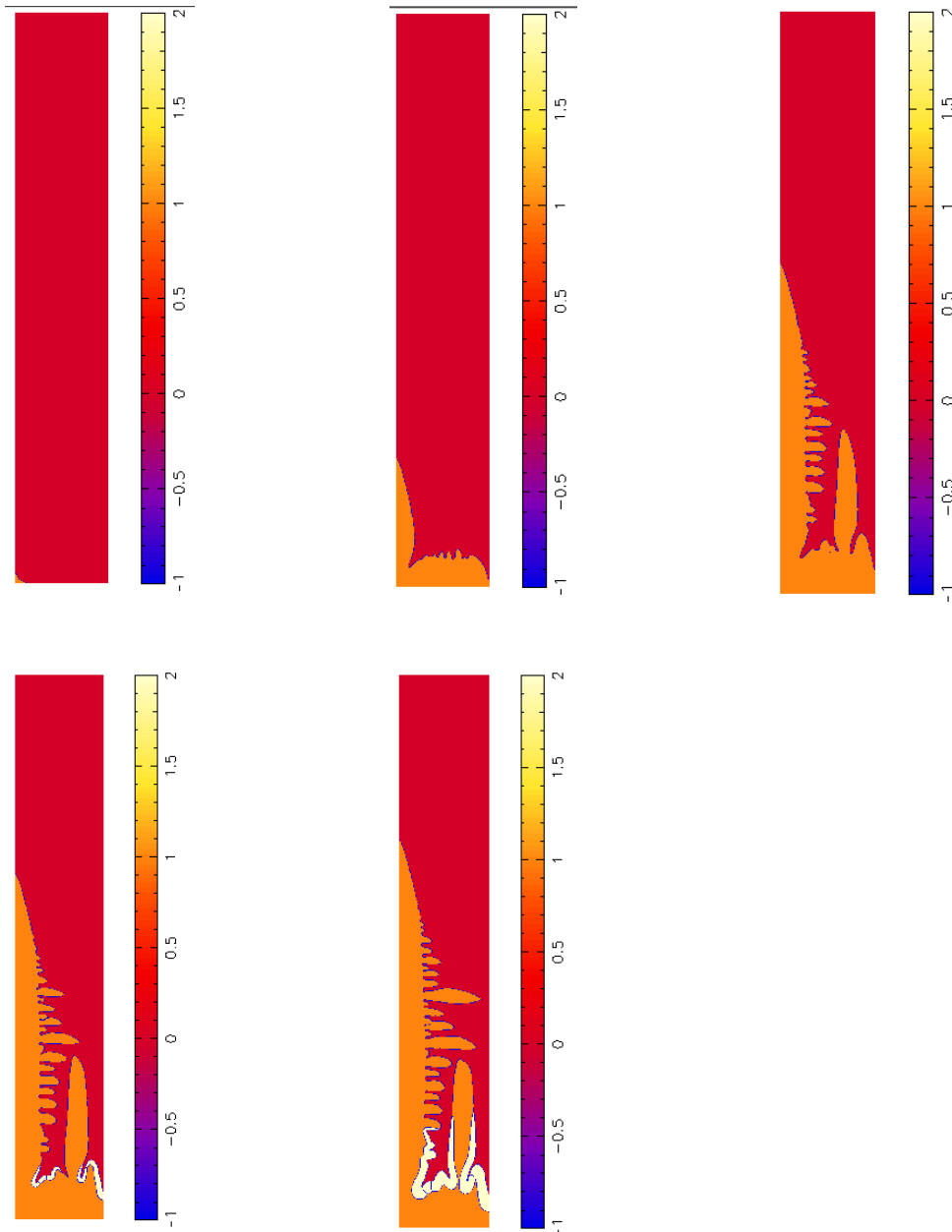


Figure 4.2. The Delta-Gamma solidification sequence at 1, 12.5, 25, 27.5 and 30 secs.

A preset δ -ferrite grain (lower left corner of upper left picture) grows dendritically in a temperature gradient (bottom cooling). A γ -austenite grain nucleates (lower left picture) and the peritectic reaction/transformation proceeds (lower row)

- Concentration of carbon (C) and Manganese (Mn)

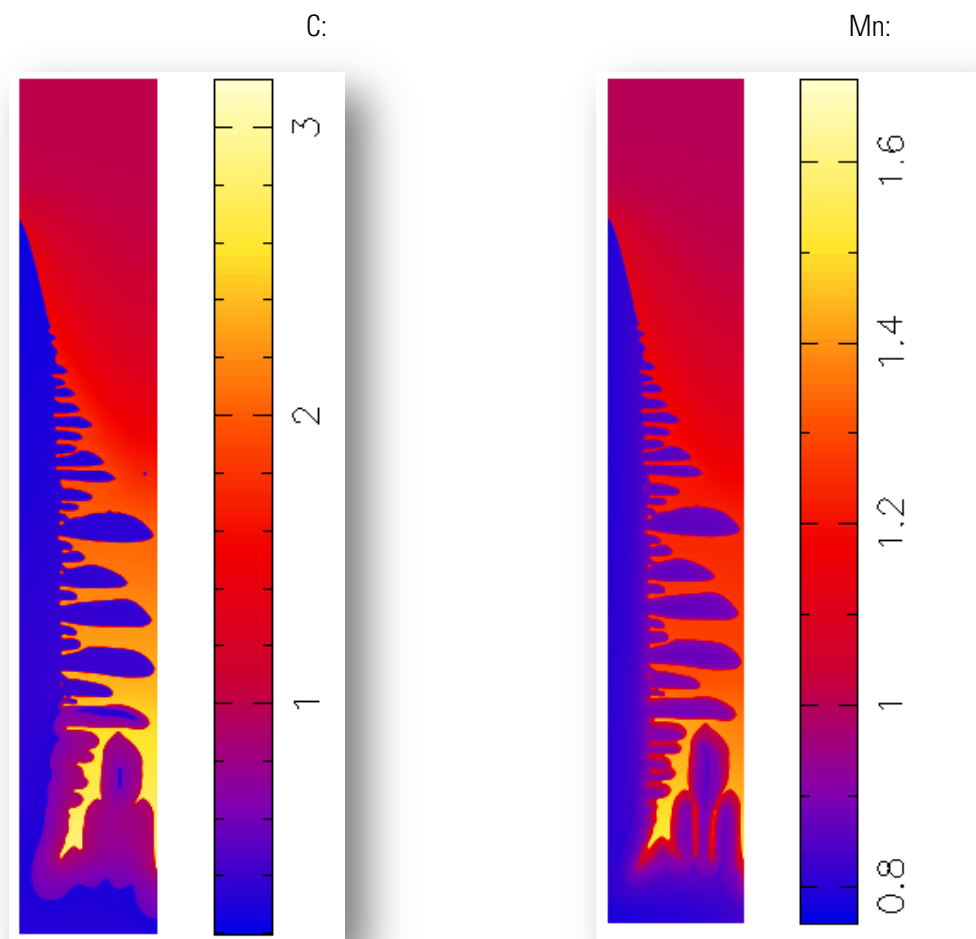


Figure 4.3 The concentrations fields for C (Delta_Gamma.conc1) and Mn(Delta_Gamma.conc2) for $t=35s$



5 “Aluminium-Copper”

5.1 Description

The three examples “Aluminium Copper” show the 2D solidification of a binary aluminium copper alloy. The “AlCu_dri” example corresponds to a directional solidification situation, whereas “AlCu_Equiaxed_dri” and “AlCu_Temp1d_dri” - describe equiaxed solidification.

All three examples are concentration-coupled with Thermo-Calc™ coupling. “AlCu_Equiaxed_dri” and “AlCu_Temp1d_dri” provide an example of the use of the “seed-density” nucleation model. Additionally “AlCu_Temp1d_dri” demonstrates the read-in of data files for temperature-dependent mobilities and latent heat as well as the use of the far field approximation for temperature coupling and release of latent heat. Another feature of this example is the use of categorized seeds.

name dri file	AlCu_dri.txt
	AlCu_Equiaxed_dri.txt
	AlCu_Temp1d_dri.txt
alloy system	Al-Cu (Al_Cu.Ges5)
composition	97 at% Al 3 at% Cu
transition	solidification

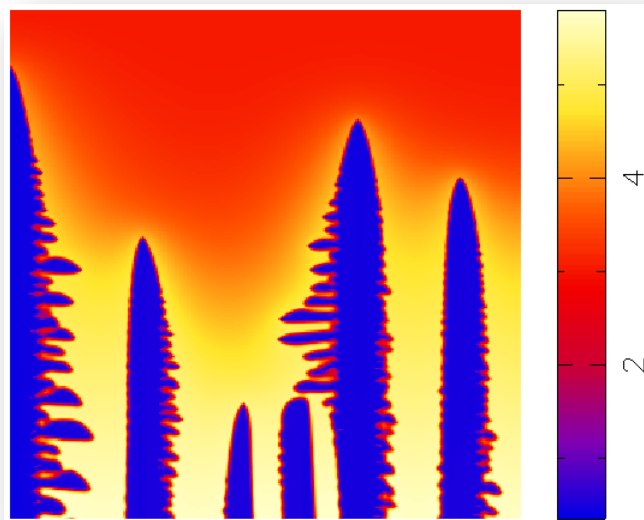


Table 4 Aluminium-Copper examples



5.2 Simulation conditions

name dri file	AlCu_dri.txt		AlCu_Equiaxed_dri.txt	AlCu_Temp1d_dri.txt
dimension	2D			
grid size	300x300 cells			200x200 cells
grid spacing	2µm			0.5µm
interface thickness	4 cells			3.5 cells
boundary conditions BCs				
phase field BCs	East:	symmetric	periodic	periodic
	West:	symmetric	periodic	periodic
	bottom:	symmetric	periodic	insulation
	top:	symmetric	periodic	insulation
concentration field BCs	East:	symmetric	periodic	periodic
	West:	symmetric	periodic	periodic
	bottom:	symmetric	periodic	insulation
	top:	fixed	periodic	insulation
solid phases:	1 solid phase: fcc_A1			2 solid phases: fcc_A1, AlCu_THETA
grain input	deterministic placement			
	1 grain of fcc_A1-phase (round r = 5; position: x = 0, z = 0; stabilisation of the grain)		0 grains at the beginning	
	further nucleation: NO		further nucleation: enabled	
	-----		seed position: bulk seed density nucleation model applied	
			integer for randomization: 13	integer for randomization: 111
			max. 1000 simultaneous nucleations	
	temperature conditions: T ₀ =912 K; G = 200 K/cm; dT/dt = -10 K/s		temperature conditions: T ₀ =915 K; G = 0 K/cm; Heat flow [J/s*cm³]: -50.000	temperature conditions: T ₀ =950K Temp-field from file
	latent heat: NO		latent heat 3D enabled	
output	files: restart, grains, phases, fraction, average fraction table, interface, driving force, mobility, curvature, interface velocity, grain time, concentration, reference phase concentration, orientation, orientation time, linearization, monitoring outputs			
				relinearisation
	times: automatic output; from 0 s to 2 s output every 0.1 s (linear step)			times: fixed output at 0.03 s; from 0.03 s to 0.05 s output every 0.003 s (linear step) from 0.05 s to 0.4 s output every 0.01 s (linear step)
special features	concentration coupling			
	1d far field diffusion approximation (30 cells, distance from the front 60 µm)		NO 1d far field diffusion approximation	
	thermodynamic coupling (GES-file: Al_Cu.GES5)			
	moving frame (distance from the upper boundary 60 µm)		NO moving frame	

Table 5 Overview of Aluminum-Copper example simulation conditions

5.3 Visualisation of the results

5.3.1 Concentration

- AlCu_dri.txt

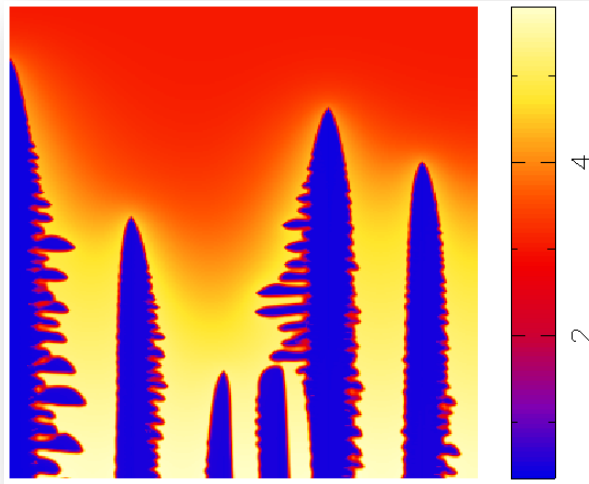


Figure 5.1. Concentration conc1 (Cu) at t=2s for driving file AlCu_dri.txt

- AlCu_Equiaxed_dri.txt

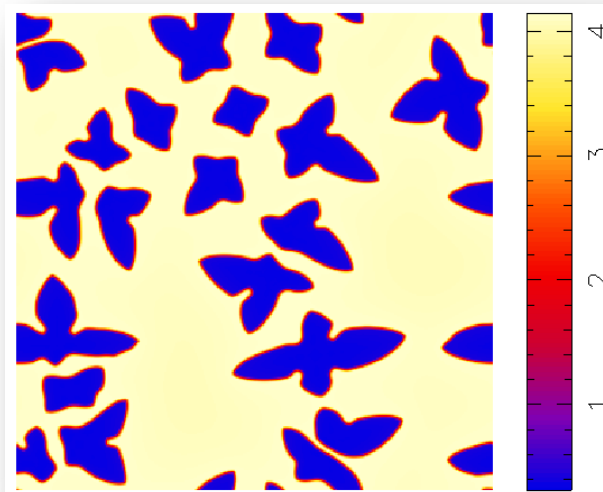
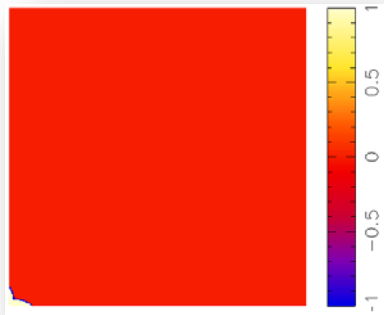


Figure 5.2. Concentration conc1 (Cu) at t=2s for driving file AlCu_Equiaxed_dri.txt

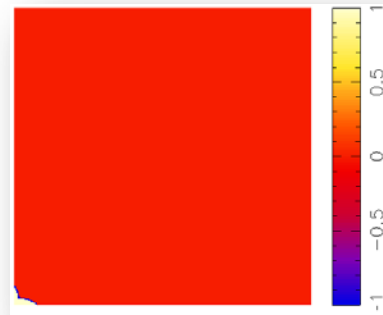


5.3.2 Solidification sequence presented by the .phas-output

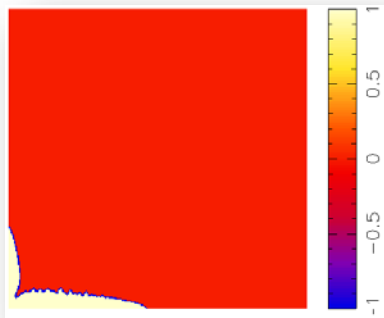
- AlCu_dri.txt (-1 → interface; 0 → liquid; 1 → fcc_A1 phase)



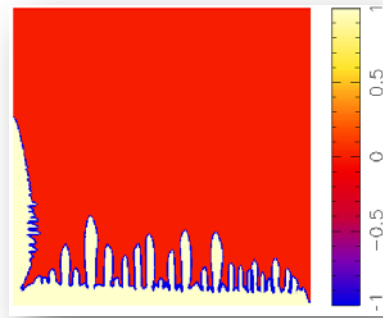
t=0s



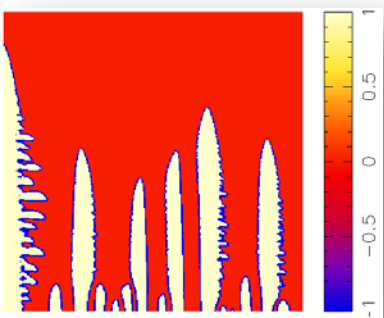
t=0.1s



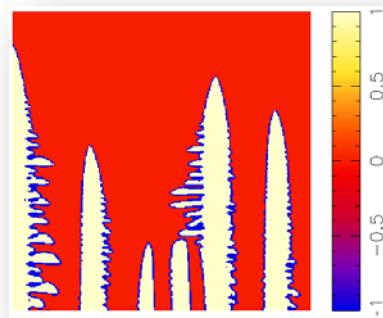
t=0.5s



t=1.0s



t=1.5s



t=2.0s

Figure 5.3. The solidification path: AlCu_dri.txt. Example:
AlCu_phas



- AlCu_Equiaxed_dri.txt (-1 → interface; 0 → liquid; 1 → fcc_A1 phase)

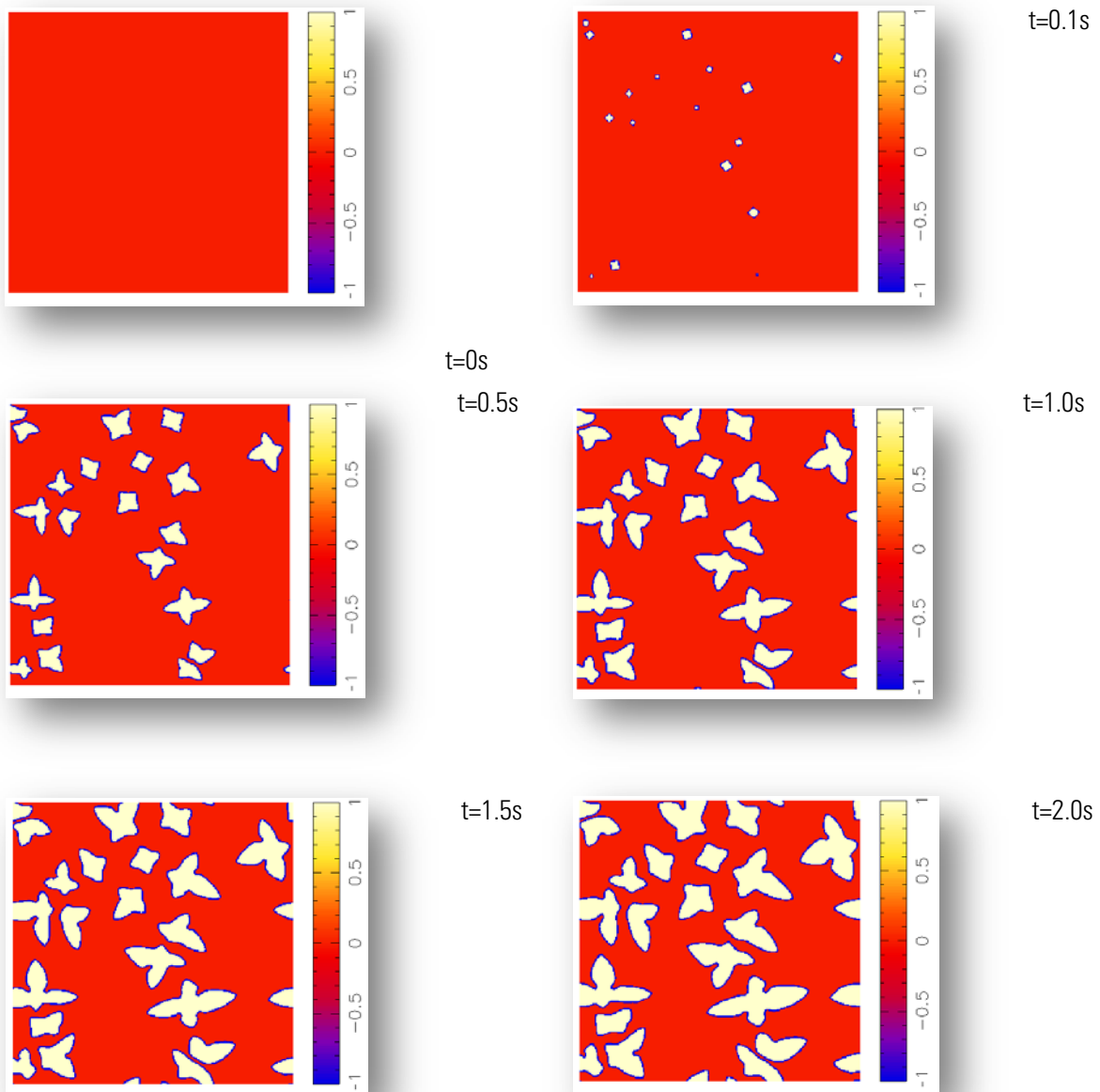
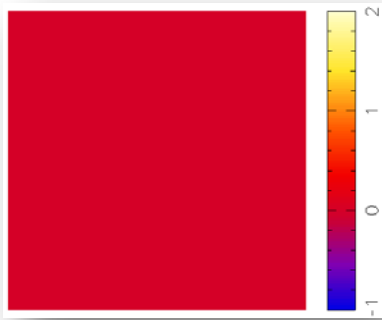


Figure 5.4. The solidification path: AlCu_Equiaxed_dri.txt.

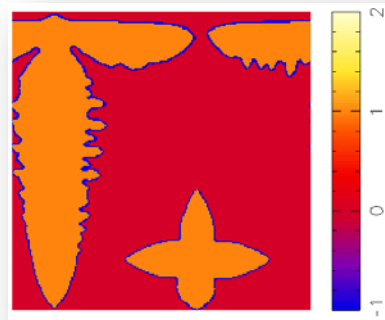
Example: AlCu_Equiaxed_phas. .

5.3.3 AlCu_Temp1d_dri.txt

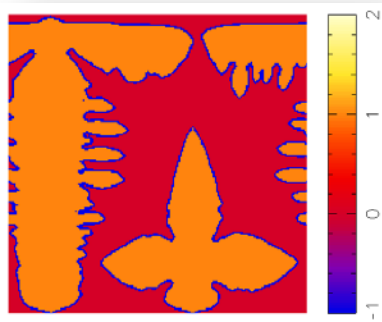
- Solidification sequence presented by the .phas-output (phase numbers: -1 → interface; 0 → liquid; 1 → FCC_A1 phase, 2 → ALCU_THETA)



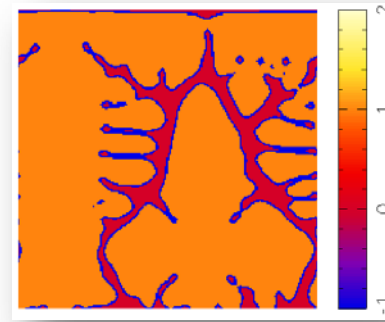
t=0s



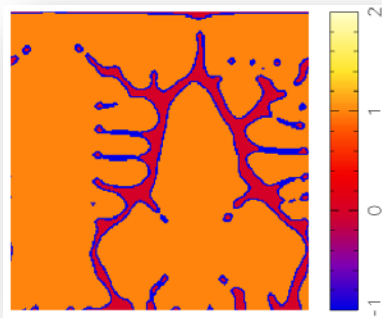
t=9.0000004E-2s



t=0.1s



t=0.3s



t=0.4s

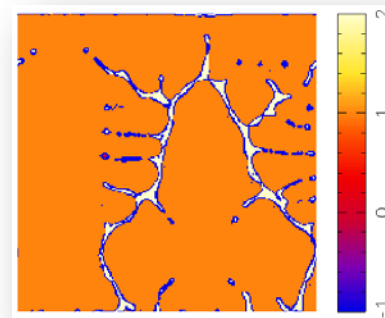


Figure 5.5. The solidification sequence for the driving file AICu_Temp1d_dri.txt



- Concentration
AlCu_Temp1d_conc1.mcr

t=0.4s

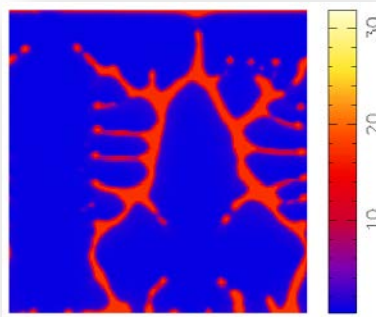


Figure 5.6. Concentration of copper after 0.4 seconds for driving file AlCu_Temp1d_dri.txt



6 “Gamma-Alpha”

6.1 Description

A series of examples (“Gamma_Alpha_dri”, “Gamma_Alpha_TQ_dri”, “Gamma_Alpha_PARA_dri”, “Gamma_Alpha_PARATQ_dri” and “Gamma_Alpha_Stress_dri”) simulates the $\gamma \rightarrow \alpha$ transformation for a ternary steel model alloy (iron, carbon and manganese). The first two examples are intended to demonstrate the difference between MICRESS® simulations with and without coupling to Thermo-Calc™. Both are concentration-coupled (either linearized phase diagrams OR database use) and demonstrate the use of the “seed-undercooling” nucleation model. Important for solid-state transformations in systems with slow and fast diffusing elements is the use of the nple (NPLe = non-partitioning, local equilibrium) redistribution model. The next two examples instead use the para-equilibrium models. The last of the examples, Gamma_Alpha_Stress_dri, shows how stress coupling can be included.

A variation of the “Gamma_Alpha_TQ_dri”-model, the “GammaAlphaCementite_LinTQ_dri”, demonstrates the application of a combination between linearized phase diagrams AND coupling to a thermodynamic database. Furthermore, cementite is added as third solid phase. Another variation of the “Gamma_Alpha_TQ_dri”-example, “GammaAlphaCementiteTQ_dri”, utilizes full coupling to a thermodynamic database. GammaAlpha_Pearlite.dri furthermore demonstrates the use of the “diffuse” effective phase model for pearlite. The main features of the individual models in the group “Gamma-Alpha” are reviewed in the next section.

name dri file	a) Gamma_Alpha_dri.txt Gamma_Alpha_TQ_dri.txt Gamma_Alpha_PARA_dri.txt Gamma_Alpha_PARATQ_dri.txt b) Gamma_Alpha_Stress_dri.txt c) GammaAlphaCementite_LinTQ_dri.txt GammaAlphaCementiteTQ_dri.txt GammaAlphaPearlite_dri.txt
alloy system	Fe-C-Mn (FeCMn.Ges5)
composition	a) 0.1 wt% C, 1.5 wt% Mn b) 0.103 wt% C, 0.49 wt% Mn c) 0.25 wt% C, 0.174 wt% Mn
transition	solid phase transition

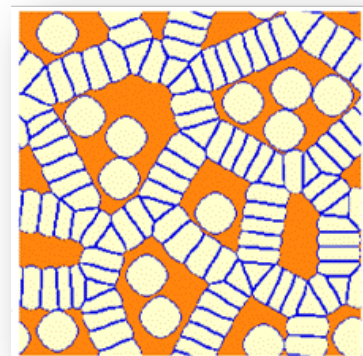


Table 6 Overview gamma-alpha examples



Group a) in Table 6 demonstrates how to use MICRESS for simulation of solid state transformations like the alpha to gamma transition. Characteristic for simulation of solid state transformations is the necessity to define an initial microstructure which is typically not needed in case of solidification. In this case, 9 initial grains of ferrite are positioned with user-defined center coordinates and radii. Voronoi construction is used to obtain a typical grain structure without overlapping or holes. The specific input data can either be chosen manually for small numbers of grains or taken from specific tools like “Random_Grid”. Alternatives for definition of initial grain structures are random generation or reading from experimental microstructures or prior MICRESS simulations.

Transformation is calculated at a constant temperature of 1023K (750 °C) where the alpha (fcc) phase is thermodynamically stable. But during the phase transformation, the dissolved elements C and Mn are redistributed, reducing the driving force for transformation. While C is a fast diffusor and can move away from the interface, Mn diffuses too slow in the time-scale of the transformation and thus must be overrun (nple) or trapped (para/paratq). This fact that the diffusion profiles of Mn cannot be spatially resolved makes it necessary to use specific models for solute redistribution which avoid artefacts of the standard redistribution model. In these examples, the conditions are chosen such that the different redistribution modes nple and para/paratq are leading to substantially different transformation rates, because in case of nple the pile-up of the element Mn in front of the moving interface is taken into account for calculation of the driving-force, while in case of para or para-tq it isn't.

The purpose of the 4 different versions of “Gamma_Alpha” is to demonstrate on one hand the differences when using linearised phase diagram data and fix Arrhenius-type diffusion coefficients versus thermodynamic and diffusion databases, and on the other hand the redistribution models nple versus para or paratq. For the first type of comparison (Gamma_Alpha_dri vs. Gamma_Alpha_TQ_dri and Gamma_Alpha_PARA_dri vs. Gamma_Alpha_PARATQ_dri) it is demonstrated how input is specified. When comparing the simulation results it turns out that there are substantial differences. The reason here is that the different redistribution modes nple and para/paraTQ lead to strongly different local tie-lines which cannot be reasonably approximated by a single linearized description. The second type of comparison (Gamma_Alpha_dri vs. Gamma_Alpha_PARA_dri and Gamma_Alpha_TQ_dri vs. Gamma_Alpha_PARATQ_dri) shows strong differences in the transformation kinetics due to the different redistribution behaviour of Mn.

It should be noted that the numerical and physical parameters used in these examples are not necessarily correct or validated by literature! The user who intends to build up own simulations based on these examples takes the full responsibility for choosing reasonable values!

Group b) in Table 6 consists of a single example and demonstrates how to include elastic stress in the simulation of the gamma-alpha transformation. Note that in this case stress is calculated only for the output time steps. The contributions to the driving force are neglected here!



Group c) in Table 6 includes cementite as a further solid phase into the simulation. The spatial resolution is adapted for the gamma-alpha reaction and thus too low for resolving individual pearlite lamellae. Two different strategies are compared how pearlite is represented: In “GammaAlphaCementite_TQ_dri”, a high number of individual cementite particles are nucleated, resembling a phase mixture with consistent phase fractions and compositions but incorrect microstructure. On the other hand, GammaAlphaPearlite_TQ uses a diffuse phase model which represents pearlite as a continuous phase mixture.

GammaAlphaCementite_LinTQ_dri is added for demonstrating how to proceed if a certain phase (cementite in this case) is not contained in the thermodynamic database. Here, only the interaction between gamma and alpha is simulated using the database while the interactions of these two phases with cementite are defined by linearized phase diagrams (in this case using the “linTQ” format).



6.2 Simulation conditions

name dri file		Gamma_Alpha_dri.txt	Gamma_Alpha_TQ_dri.txt	Gamma_Alpha_PARA_dri.txt	Gamma_Alpha_PARA_dri.txt	Gamma_Alpha_Cementite_LinTQ_dri.txt	Gamma_Alpha_CementiteTQ_dri.txt	Gamma_Alpha_PearliteTQ_dri.txt	Gamma_Alpha_Stress_dri	
dimension		2D							3D	
grid size (cells)		250x1x250							50x20x50	
grid spacing		0.25μm							0.5μm	
interface thickness (cells)		3						3.5	4	
boundary conditions BCs										
phase field BCs	East:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
	West:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
	North:	---	---	---	---	---	---	---	insulation	
	South:	---	---	---	---	---	---	---	insulation	
	bottom	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
	top:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
concentra tion field BCs	East:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
	West:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
	North:	---	---	---	---	---	---	---	insulation	
	South:	---	---	---	---	---	---	---	insulation	
	bottom:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
	top:	periodic	periodic	periodic	periodic	periodic	periodic	periodic	periodic	
solid phases:		2 solid phases: γ , α				3 solid phases: γ , α , cementite				
grain input		<u>deterministic</u>				<u>random:</u>				
		placement of 9 grains of α -phase (round)				8 grains of one type of grains (round)				
		stabilisation of the grains); Voronoi construction								12 grains of one type of grains (round)
		<u>further nucleation:</u> enabled								
		seed types:3				seed types:4			seed types:3	



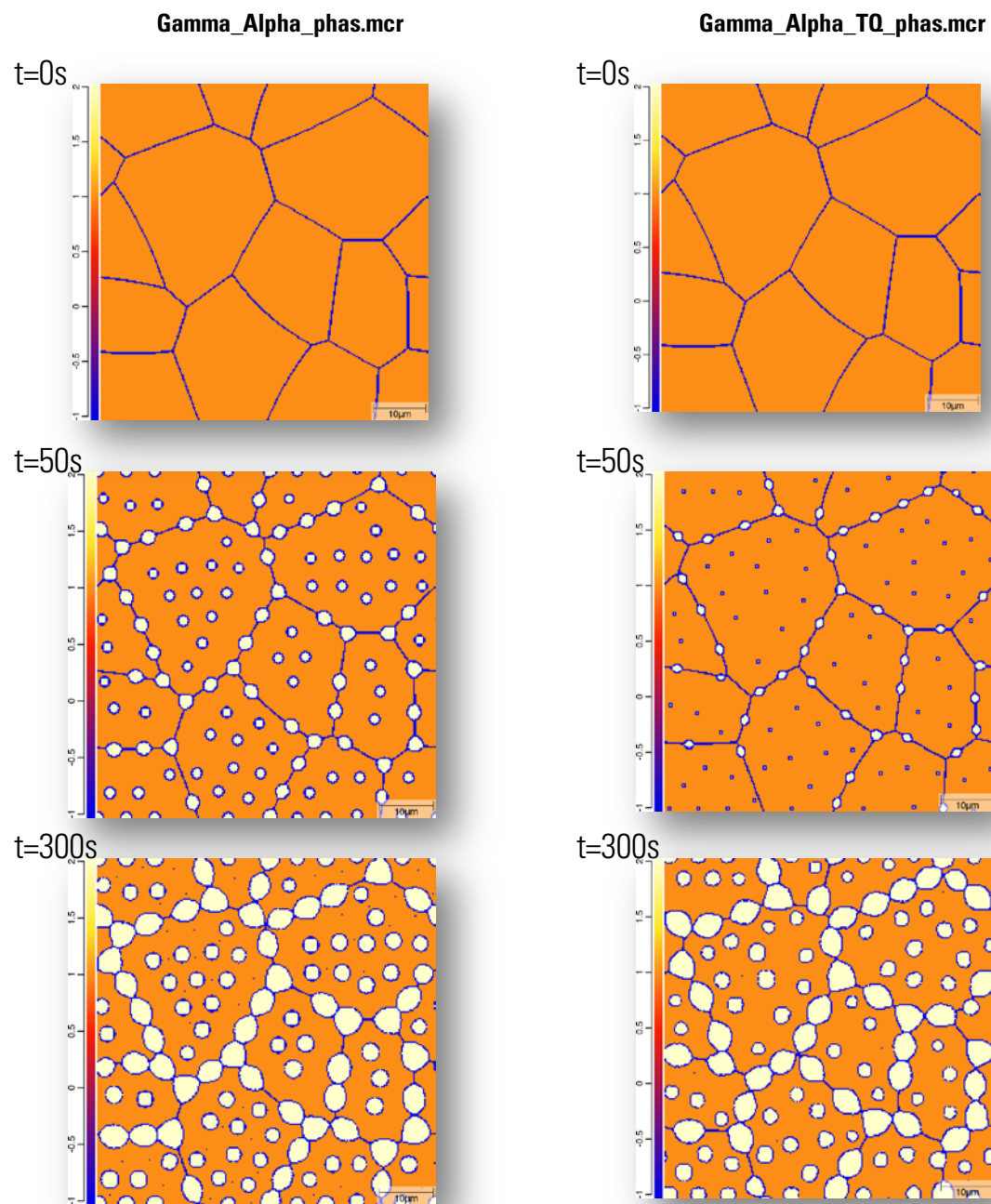
	seed positions: triple, interface, bulk					seed positions: triple, interface	
	seed undercooling nucleation model applied						
	simultaneous nucleation: automatic						
	<u>temperature conditions:</u> T ₀ =1023 K; G = 0 K/cm; dT/dt = 0 K/s				<u>temperature conditions:</u> T ₀ =1030 K; G = 0 K/cm; dT/dt = -10 K/s		<u>temperature conditions:</u> T ₀ =1095 K; G = 0 K/cm
	latent heat: NO						
output	files: restart, grains, phases, average fraction table, interface, driving force, grain time, concentration, reference phase concentration, monitoring outputs						normal stress, von Mises stress output, displacement data
	<u>times:</u> from 01.0 s to 6 s output every 1.0s (linear step) from 06.0 s to 10 s output every 2.0s (linear step) from 10.0 s to 30 s output every 5.0s (linear step) from 30.0 s to 100 s output every 10.s (linear step) from 100 s to 300 s output every 25.s (linear step)				<u>times:</u> output at 00.25 and 01.00 s from 01.00 s to 10 s output every 0.5 s (linear step) from 10.00 s to 35 s output every 1 s (linear step)		<u>times:</u> output at 5, 10 and 15 s
special features	concentration coupling						concentration and stress coupling
	NO 1d far field diffusion approximation						
	no thermodynamic coupling	thermodynamic coupling: enabled	no thermodynamic coupling	thermodynamic coupling: enabled			no thermodynamic coupling
		FECMn.Ges5		FECMn.Ges5			
		database global		database global	linearTQ	database global	
	NO moving frame						

Table 7 GammaAlpha Examples: Overview of simulation conditions/ parameters



6.3 Visualisation of the results

6.3.1 Gamma_Alpha_dri and Gamma_Alpha_TQ_dri





C-composition after 50 s

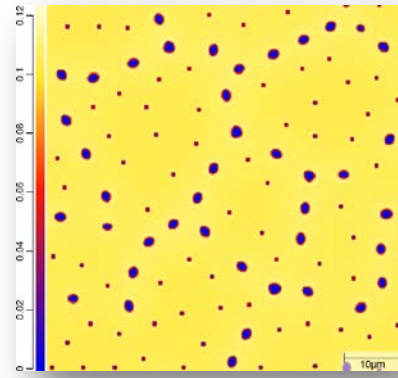
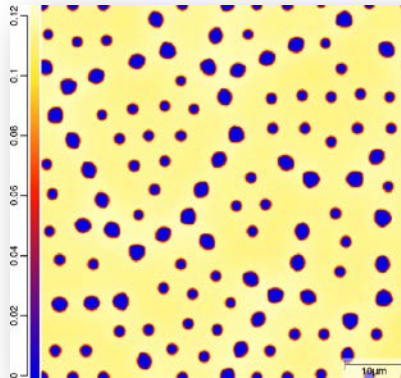
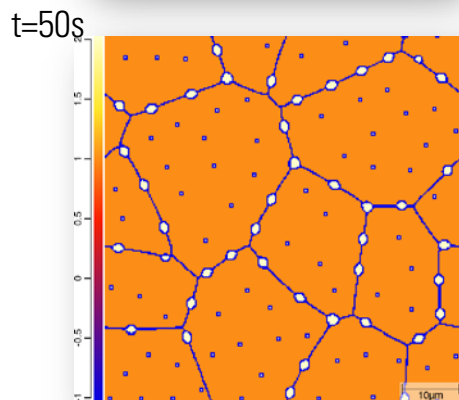
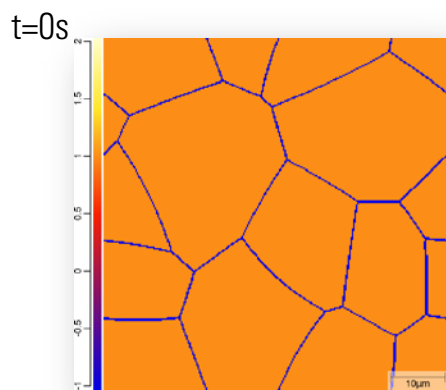
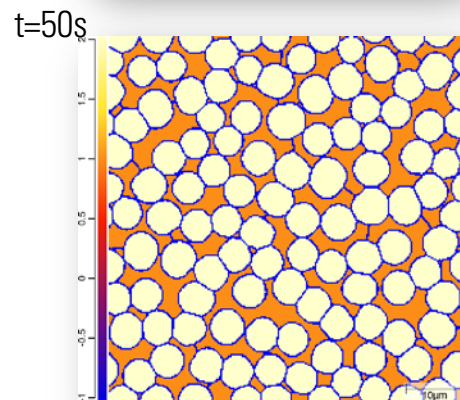
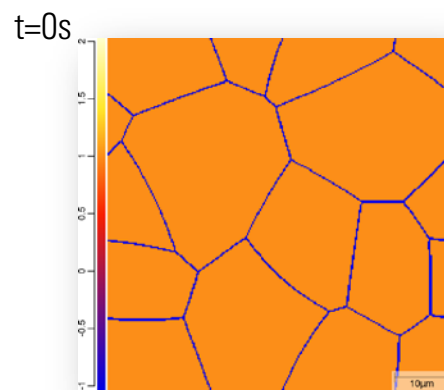


Figure 6.1. The phase transition sequence for the driving files: Gamma_Alpha_dri.txt and Gamma_Alpha_TQ_dri.txt

Gamma_Alpha_TQ_phas.mcr

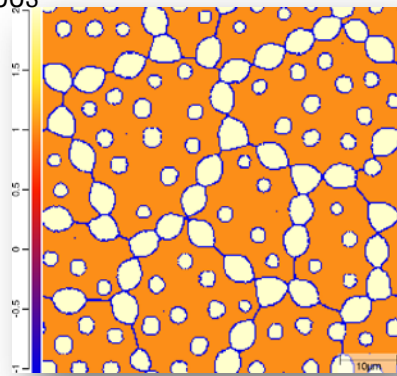


Gamma_Alpha_PARATQ_phas.mcr

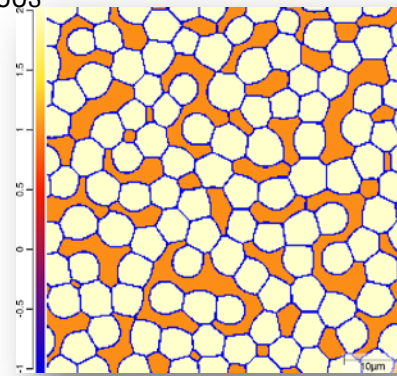




t=300s



t=300s



C-composition after 50 s

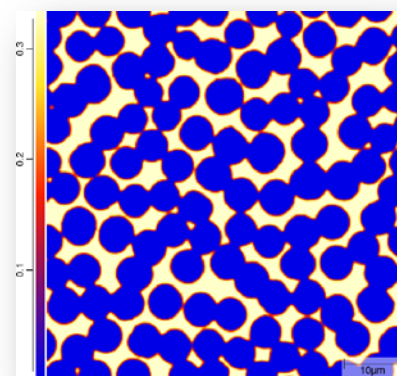
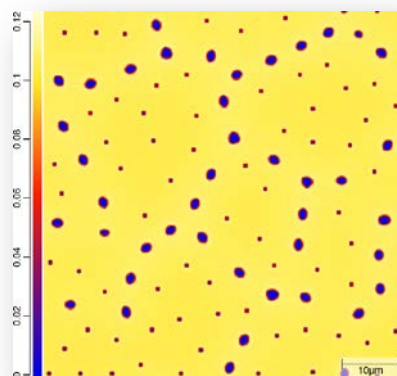


Figure 6.2. The phase transition sequence for the driving files:
Gamma_Alpha_TQ_dri.txt and Gamma_Alpha_PARATQ_dri.txt



6.3.2 GammaAlpha_Cementite_LinTQ_dri and _Cementite_TQ_dri

Phase transition path presented by the .phas-output. **Note:** Same results, but different colour codes used for the output! (-1 red interface; 0 not assign → gamma; 2 alpha; 3 cementite)

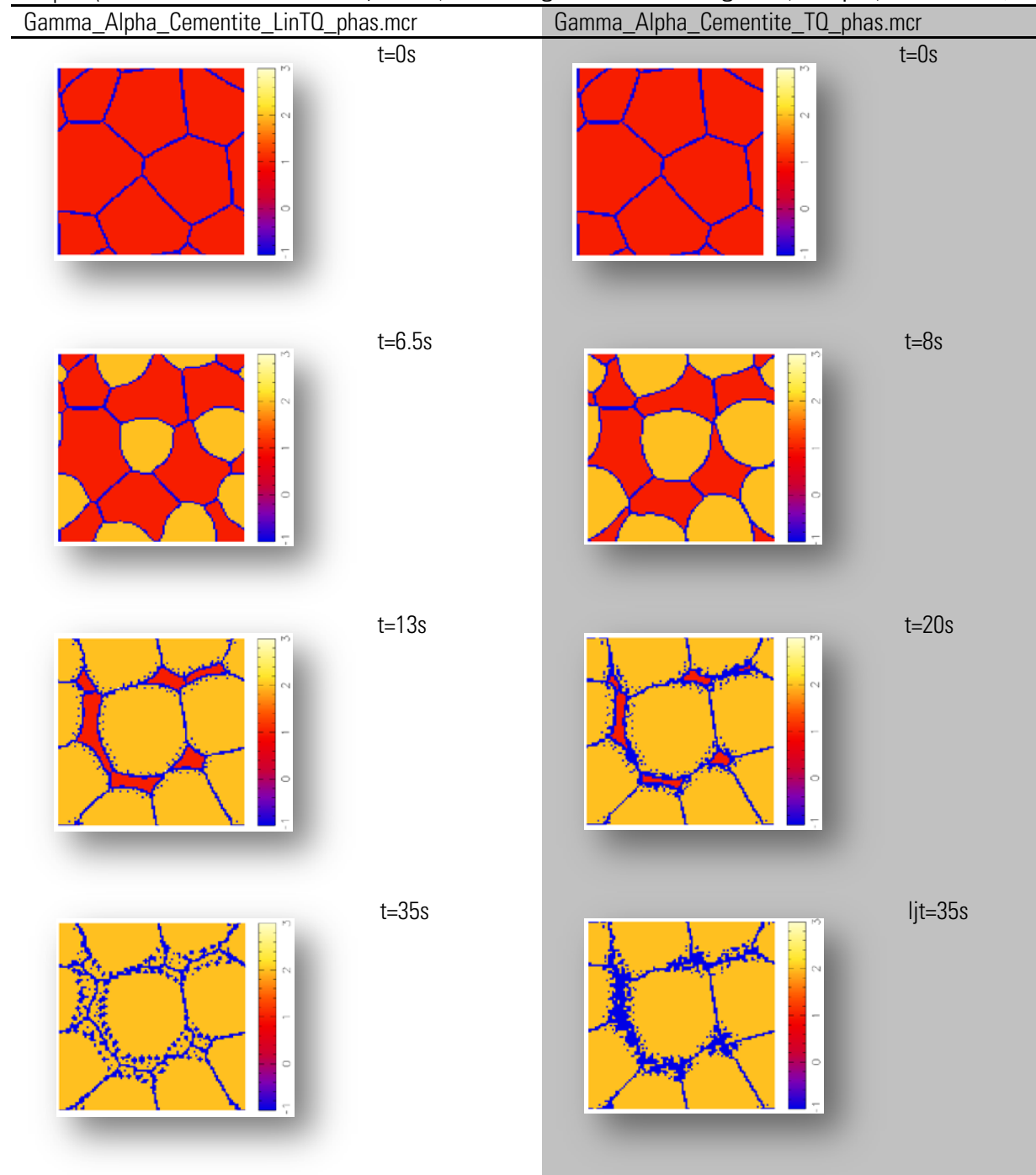


Figure 6.3. The phase transition path: GammaAlpha_Cementite_LinTQ_dri and GammaAlpha_CementiteTq_dri



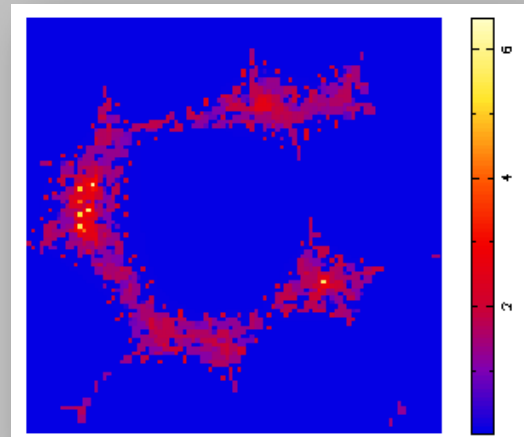
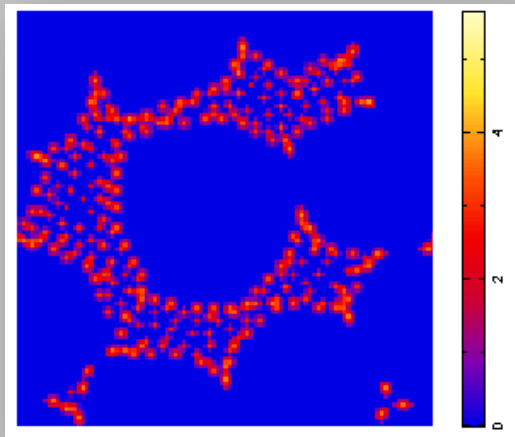
- Concentration

Gamma_Alpha_Cementite_LinTQ_in.txt,
Concentration

Carbon

Gamma_Alpha_CementiteTQ_in.txt,
Concentration

Carbon



Gamma_Alpha_Cementite_LinTQ_in.txt, Manganese
concentration

Gamma_Alpha_CementiteTQ_in.txt,
Manganese concentration

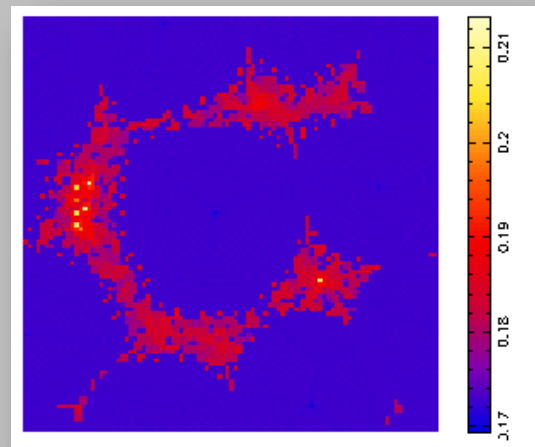
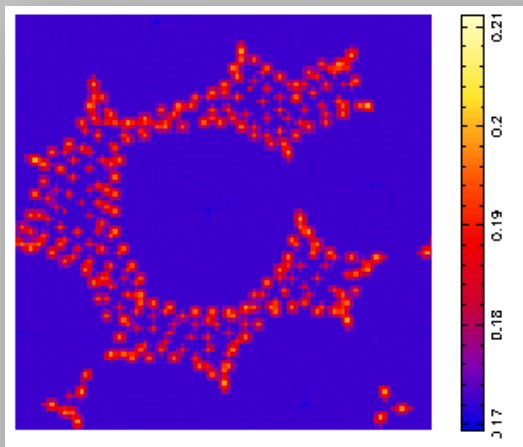


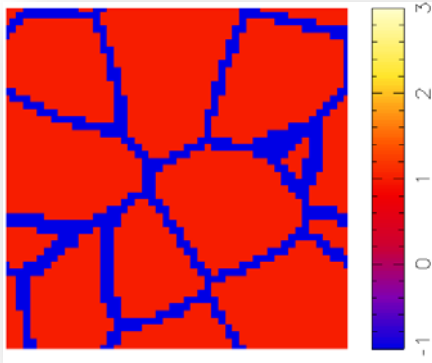
Figure 6.4. Concentration: “Gamma-Alpha_Cementite” with linearized (LinTQ) and non-linearised (TQ) concentration-coupling (time step 35 sec in both cases)



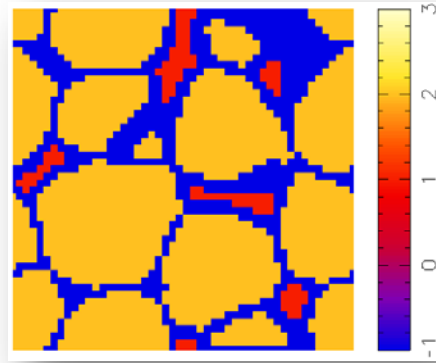


6.3.3 Gamma_Alpha_Stress_dri

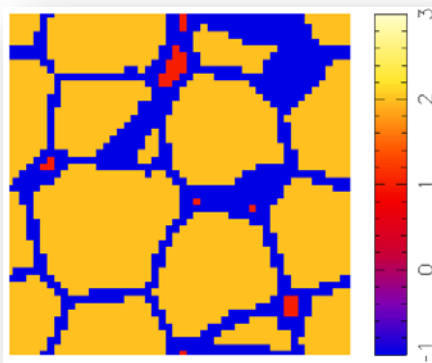
- Transformation sequence presented by the .phas-output (-1 interface; 0 not assigned, 1 gamma; 2 alpha; 3 cementite)



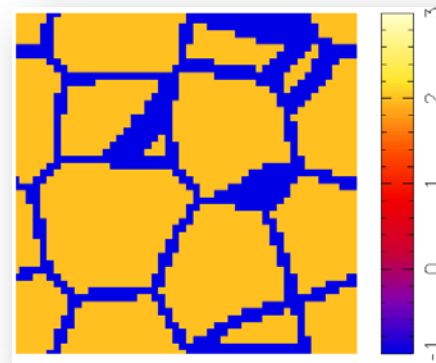
t=0s



t=6s



t=10s

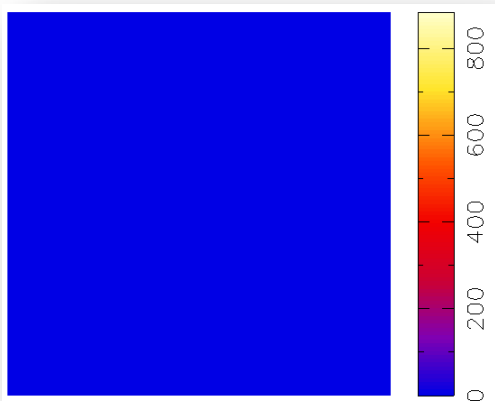


t=15s

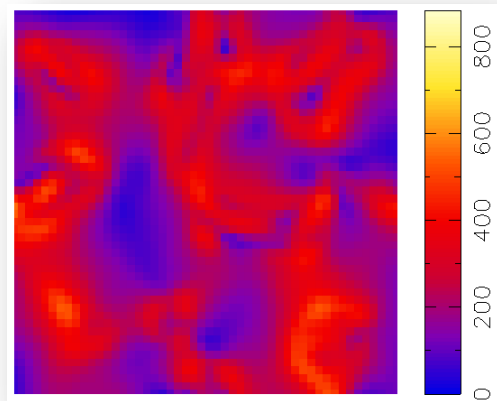
Figure 6.5. The phase transition sequence: Gamma_Alpha_Stress_in.txt



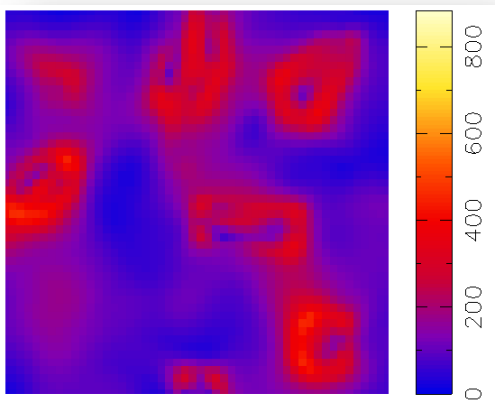
- Von Mises stress



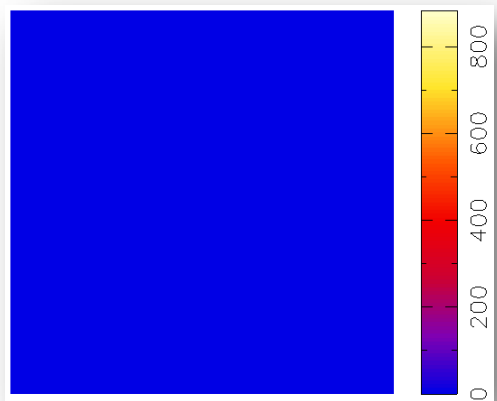
t=0s



t=5s



t=10s



t=15s

Figure 6.6. Equivalent stresses for the “Gamma-Alpha_Stress” example



7 “Grain-Growth”

7.1 Description

The group of examples “Grain Growth” (“Grain_Growth_dri”, “Grain_Growth_Particle_Pinning_dri” and “Grain_Growth_Solute_Drag_dri” shows how MICRESS® can be used without coupling to external fields like temperature or concentration, i.e. using only the curvature as a driving force for the transformation. Respective curvature based coarsening is inherent to phase-field models. These examples show how to read-in initial microstructures. The “Grain_Growth_dri” example displays “pure” grain growth, whereas the other examples draw on specific models hindering grain boundary motion like e.g. the particle-pinning, the solute-drag and KTH-solute-drag models, respectively

In addition, grain growth with non-linear temperature profiles is modeled in the „Grain_Growth_Profiles_dri” example. The example “Grain_Growth_Solute_Drag_dG_in.txt” is the same as “Grain_Growth_Solute_Drag_in.txt” apart from the mobility which is not constant but dependent on the driving force.

name dri file	Grain_Growth_in.txt Grain_Growth_Particle_Pinning_in.txt Grain_Growth_Profiles_in.txt Grain_Growth_Solute_Drag_dG_in.txt Grain_Growth_Solute_Drag_in.txt
alloy system	not specified e.g. steel
composition	not specified e.g. austenite
modelled phenomenon	grain growth with/without pinning

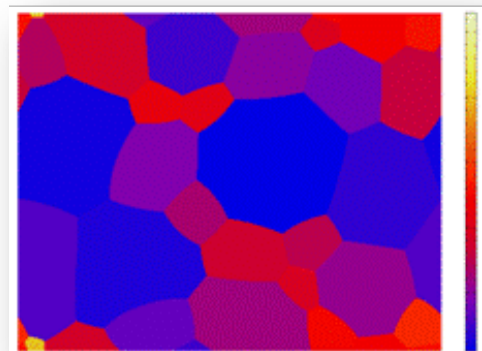


Table 8 Examples: Grain-Growth details



7.2 Simulation conditions

name dri file		Grain_Growth_in.txt	Grain_Growth_Particle_Pinning_in.txt	Grain_Growth_Solute_Drag_in.txt	Grain_Growth_Solute_Drag_dG_in.txt	Grain_Growth_Profiles_in.txt
dimension		2D				
grid size (cells)		400x1x320				100x1x500
grid spacing		1.5µm				
interface thickness (cells)		5				
boundary conditions BCs						
phase field BCs	East:	periodic	periodic	periodic	periodic	periodic
	West:	periodic	periodic	periodic	periodic	periodic
	bottom	periodic	periodic	periodic	periodic	periodic
	top:	periodic	periodic	periodic	periodic	periodic
solid phases:		1 solid phases				
grain input		<u>from file:</u> Grain_Growth_Microstructure.txt				<u>random</u> : integer randomization: 123; 100 different round grains with stabilisation and voronoi construction
		<u>further nucleation:</u> NO				
		<u>phase interaction:</u> pure	<u>phase interaction:</u> with particle pinning	<u>phase interaction:</u> with solute drag	<u>phase interaction:</u> pure	
		<u>mobility:</u> constant			<u>mobility:</u> dg_dependent Grain_Growth_dG_Mobility_Data	<u>mobility:</u> temperature dependent
		<u>temperature conditions:</u> T ₀ =1000 K; G = 0 K/cm; dT/dt = 0 K/s (isothermal)				from file



output	files: restart, grains, phases, interface, mobility, curvature, velocity, grain-time file, von Neumann Mullins output, monitoring outputs				
	times: from 0.00 s to 20 s output every 5 s (linear step) from 20.00 s to 250 s output every 10 s (linear step) from 250.00 s to 1000 s output every 50 s (linear step)			times: from 0.00 s to 0.4 s output every 0.02 s (linear step) from 0.4 s to 1 s output every 0.05 s (linear step)	
special features	phase field coupling				
	no thermodynamic coupling				
	microstructure read in from file Grain_Growth_Microstructure.txt				
	NO moving frame				
				driving force dependent mobility	temperature dependent mobility -> temperature trend read in from file

Table 9 Example: Grain Growth: field parameters



7.3 Visualisation of the results

7.3.1 Pure grain growth and grain growth with particle pinning and solute drag

- Grain growth sequence presented by the .korn-output (each grain has a different colour)

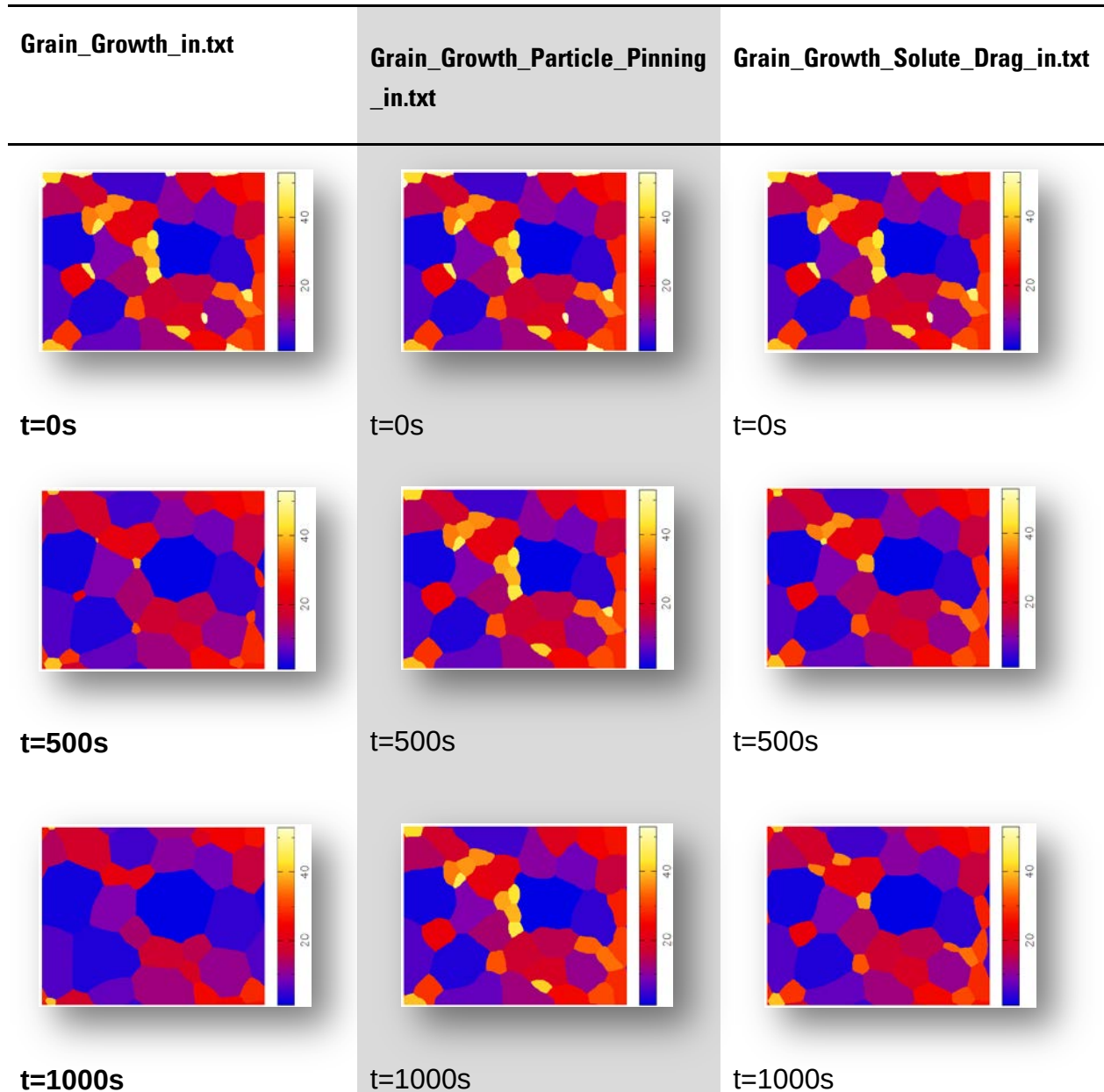
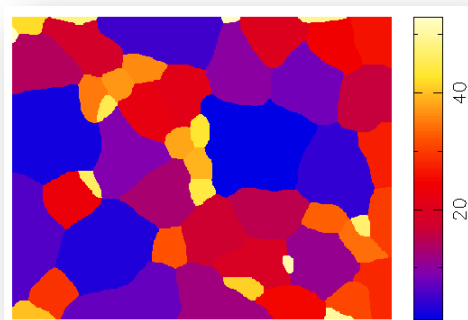


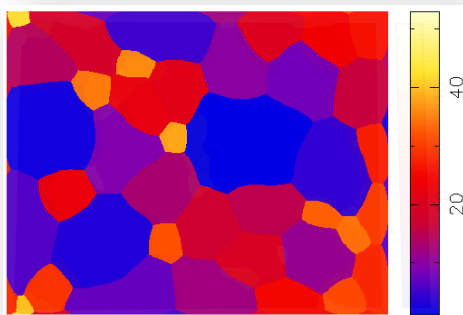
Figure 7.1. Grain growth sequence presented by the .korn-output (each grain has a different colour)



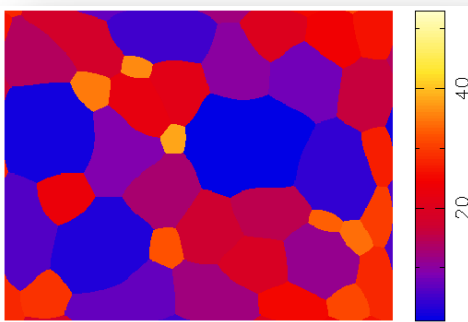
7.3.2 Grain_Growth_Solute_Drag_dG_in.txt



$t=0s$



$t=500s$



$t=1000s$

Figure 1. The grain growth sequence with driving force dependent mobility (Grain_Growth_Solute_Drag_dG_korn.txt)



7.3.3 Grain_Growth_Profiles_in.txt

- Grain growth: Grain_Growth_Profiles_korn.txt

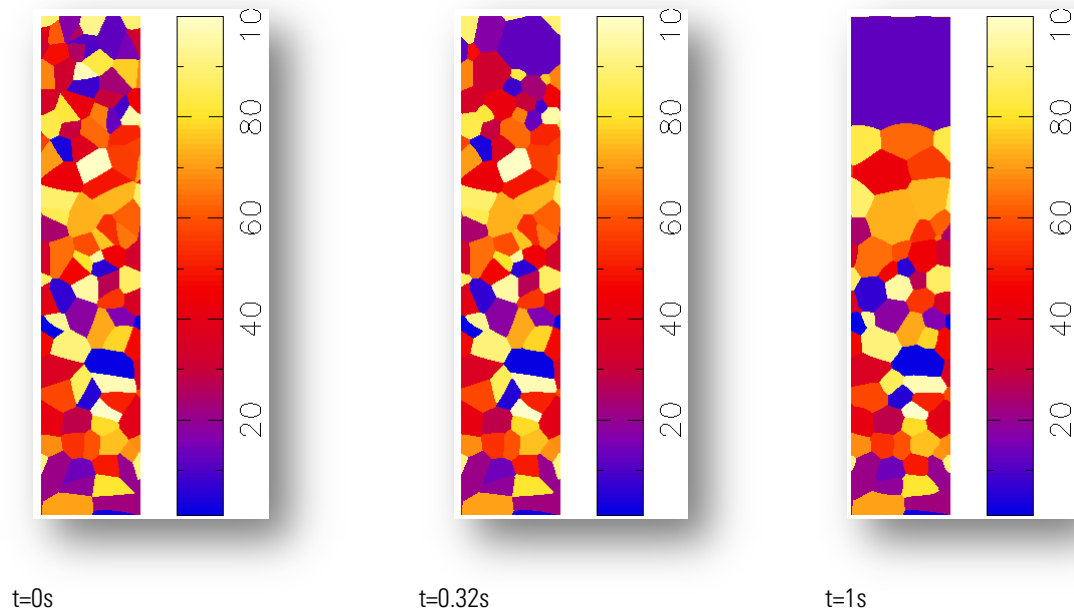


Figure 2. The grain growth path with temperature dependent mobility



- Temperature distribution: Grain_Growth_Profiles_temp.txt

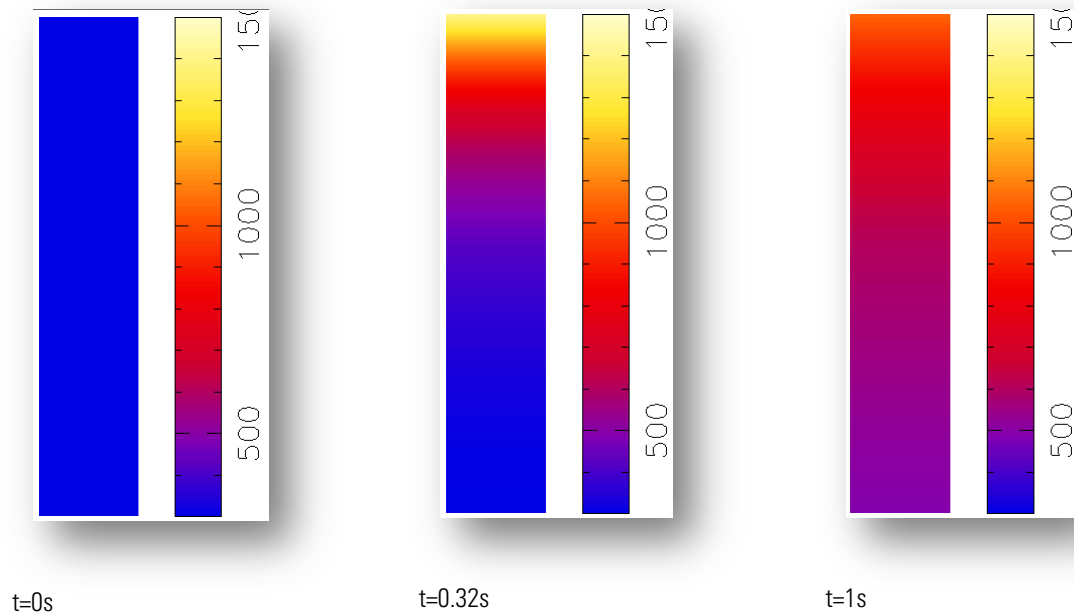


Figure 3. The temperature profiles for different time steps



8 “Phosphorous Peak”

8.1 Description

These two examples, “P_Peak_1D_dri” and “P_Peak_2D_dri” show full multicomponent diffusion with coupling to Thermo-Calc™ using industrial steel grades. The first example is one-dimensional and provides a ready benchmark against DICTRA™.

name dri file	P_Peak_1D_in.txt P_Peak_2D_in.txt
alloy system	Fe-C-Mn-Si-P (Fe_C_Mn_Si_P.Ges5)
composition	0.4 wt% C 0.8 wt% Mn 0.7 wt% Si $3 \cdot 10^{-2}$ wt% P
transition	solidification

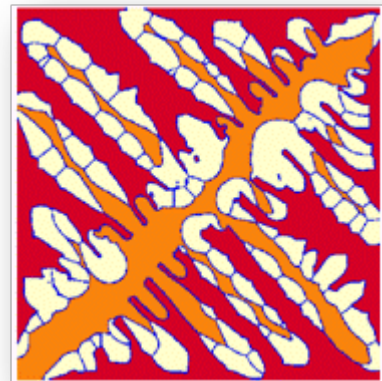


Table 10 Example: Phosphorous Peak details: modelled phases are liquid(red), ferrite(orange) and austenite (bright)



8.2 Simulation conditions

name dri file		P_Peak_1D_in.txt	P_Peak_2D_in.txt
dimension		1D	2D
grid size (cells)		1x1x200	400x1x400
grid spacing		0.5µm	2µm
interface thickness (cells)		5	4
boundary conditions BCs			
phase field BCs	east:	insulation	symmetric
	west:	insulation	symmetric
	bottom	insulation	periodic
	top:	insulation	periodic
concentration field BCs	east:	insulation	periodic
	west:	insulation	periodic
	bottom:	insulation	periodic
	top:	insulation	periodic
solid phases:		2 solid phases: BCC_A2 (ferrite), FCC_A1 (austenite)	
grain input		<u>deterministic</u> placement of 1 grain (round, coordinates: x=0.25, z=0.25, r=0), stabilisation of the grains); no voronoi construction	
		rotation angle 0°	rotation angle 45°
		Max. number of new nuclei: 1	Max.number of new nuclei: 250
		<u>further nucleation</u> : enabled	
		seed types:1, seed position: interface	
			simultaneous nucleations: automatic
temperature		<u>temperature conditions</u> : $T_0=1763.75$ K; $G = 0$ K/cm; $dT/dt = -0.2$ K/s	
		<u>latent heat</u> : NO	



output	files: restart, grains, phases, average fraction table, concentration, concentration of the reference phase, average concentration per phase, linearization output, monitoring outputs	
	<u>times:</u> from 00.00 s to 700 s output every 50 s (linear step) from 700 s to 2500 s output every 100 s (linear step)	<u>times:</u> from 00.00 s to 160 s output every 10 s (linear step) from 160 s to 170 s output every 2.5 s (linear step) from 170 s to 200 s output every 10 s (linear step) from 200 s to 600 s output every 50 s (linear step) from 600 s to 3000 s output every 100 s (linear step)
special features	concentration coupling	
	NO 1d far field diffusion approximation	
	thermodynamic coupling: enabled; Fe_C_Mn_Si_P.Ges5 datafile	
	NO moving frame	

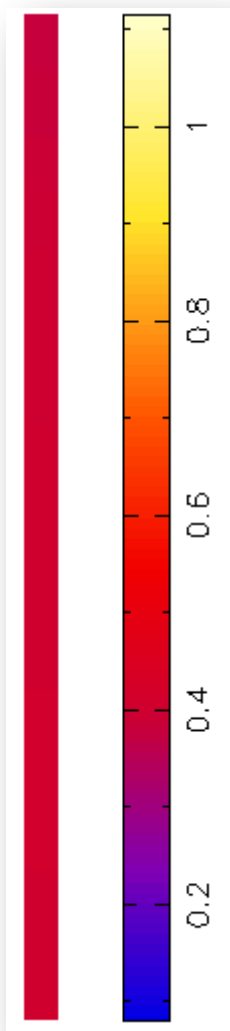
Table 11 Example: Phosphorus Peak: field parameters



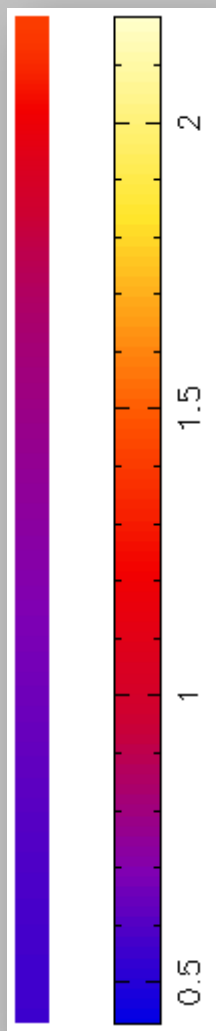
8.3 Visualisation of the results

8.3.1 P_Peak_1D_in.txt

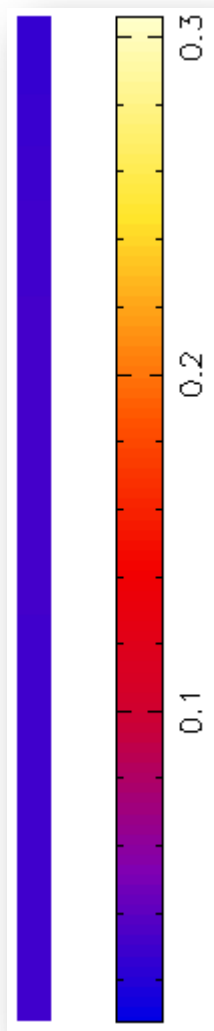
P_Peak_1D_conc1



P_Peak_1D_conc2



P_Peak_1D_conc3



P_Peak_1D_conc4

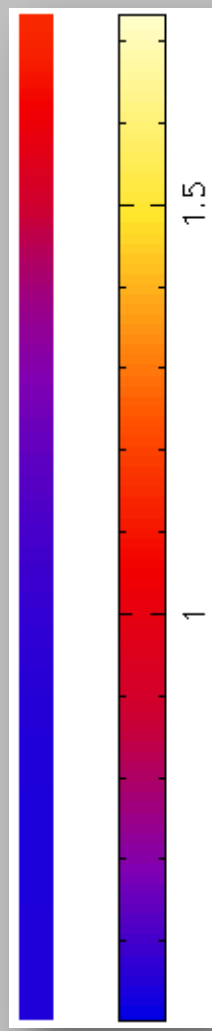


Figure 4. The 1D concentration field: P_Peak_1D_conc1.mcr to P_Peak_1D_conc4.mcr (1:C, 2:Mn, 3:P and 4: Si) for $t=2000s$.



8.3.2 P_Peak_2D_in.txt

- Solidification sequence presented by the .phas-output (-1 → interface; 0 → liquid, 1 → BCC_A2 (ferrite), 2 → FCC_A1 (austenite))

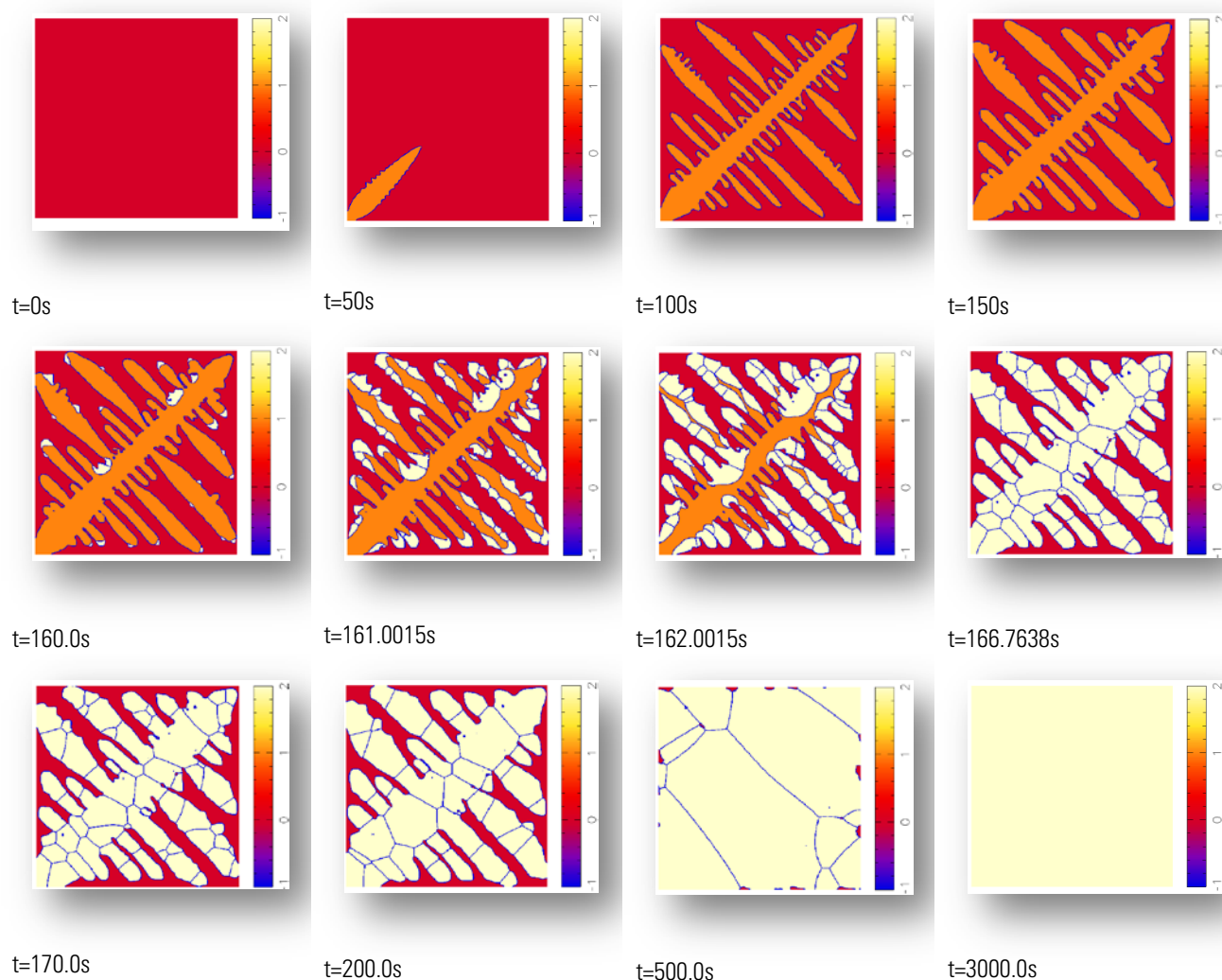


Figure 5. The solidification path: P_Peak_2D_phas.mcr



- Concentration evolution presented for the .conc2 (Mn)

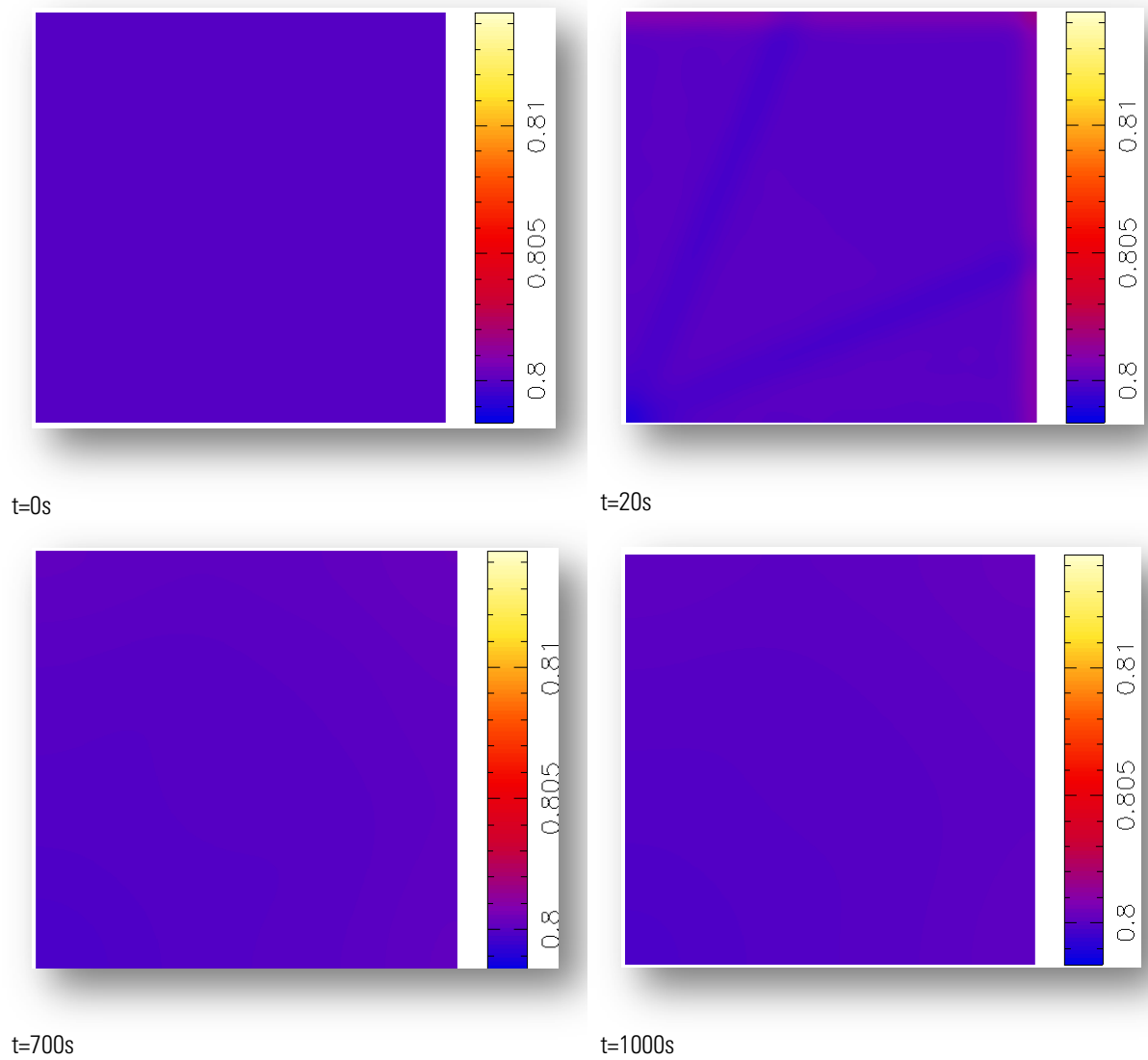


Figure 8.3. The concentration field for Manganese: P_Peak_2D_conc2.mcr (Mn) (1: C, 2: Mn, 3: P and 4: Si)



9 “Recrystallisation”

9.1 Description

The five examples, “ReX_1_dri”, “ReX_2_dri”, “ReX_3_dri”, “ReX_4_dri”, and “ReX_5_dri” illustrate various topics related to recrystallisation. All examples show the influence of misorientation and stored-energy on recrystallisation/growth and the use of the Voronoi criterion. In addition, “ReX_1_dri” and “ReX_5_dri” demonstrate the use of the “seed-undercooling” nucleation model.

name dri file	ReX_1_in.txt ReX_2_in.txt ReX_3_in.txt ReX_4_in.txt ReX_5_in.txt
alloy system	Not specified: e.g. steel
composition	Not specified: e.g. ferrite or austenite
phenomenon	recrystallisation

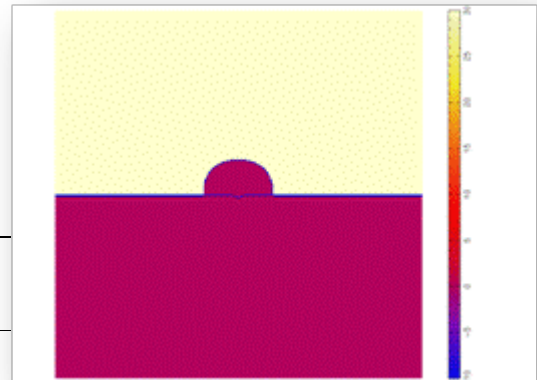


Table 12 Example Recrystallisation: details



9.2 Simulation conditions

name dri file		ReX_1_in.txt	ReX_2_in.txt	ReX_3_in.txt	ReX_4_in.txt	ReX_5_in.txt
dimension		2D				
grid size (cells)		400x1x400	500x1x500	400x1x400	500x1x300	500x1x1000
grid spacing		0.25µm	0.5µm	2E-02µm	0.5µm	
interface thickness (cells)		5		4	5	
boundary conditions BCs						
phase field BCs	east:	insulation	insulation	periodic	insulation	periodic
	west:	insulation	insulation	periodic	insulation	periodic
	bottom	insulation	insulation	insulation	insulation	insulation
	top:	insulation	insulation	insulation	insulation	insulation
solid phases:		1 solid phase: different stored energy assigned to different grains				
grain input		<u>deterministic</u>		<u>random</u> : integer for randomization: 13	<u>deterministic</u>	<u>random</u> : integer for randomization: 6
		3 new grains (round)	6 new grains (round)	two types of grains (type 1: 100, type 2: 30)	22 new grains (elliptic)	4 types of grains (type 1: 5, type 2: 5, type 3: 15, type 4: 5); elliptic
		stabilisation				
		Voronoi construction				
		<u>further nucleation</u> : NO	<u>further nucleation</u> : YES	<u>further nucleation</u> : NO	<u>further nucleation</u> : YES	<u>further nucleation</u> : YES
		<u>phase interaction</u> :pure <u>mobility</u> :constant				
		<u>recrystallisation</u> : phase 1: anisotropic cubic symmetry				
			<u>misorientation</u>			
			3 types of seeds; position of the seeds: interface, triple, bulk; seed undercooling nucleation model applied; maximum number of		2 types of seeds; position of the seeds: interface, region; seed undercooling nucleation model applied; maximum number of	2 types of seeds; seed position: interface, region; stabilisation; maximum number of simultaneous nucleations: 5



		simultaneous nucleations: 10		simultaneous nucleations: 25	
	<u>temperature conditions:</u> T ₀ =1000 K; G = 0 K/cm; dT/dt = 0 K/s			<u>temperature conditions:</u> T ₀ =1000 K; G = 0 K/cm; dT/dt = -1 K/s	
	<u>latent heat:</u> NO				
output	<u>files:</u> phases, interface, recrystallisation, recrystallized fraction output, orientation		<u>files:</u> orientation	<u>files:</u> grain number output	<u>files:</u> recrystallisation, miller indices, orientation
	linear step output; output at 0.2 and 2.2 s		linear step output; output at 0.05 and 0.6 s	output from 0 to 10s every 0.5 s output from 10 s to 15 s every 1 s output from 10 s to 30 s every 5 s output from 20 to 270 s every 30 s (linear step)	output from 0 to 5s every 0.5 s output from 5 s to 10 s every 1 s output from 10 s to 20 s every 2 s output from 20 to 30 s every 50 s (linear step)
special features	phase field coupling				
	no thermodynamic coupling				
	NO moving frame				

Table 13 Example: Recrystallisation: simulation conditions



9.3.1 Visualisation of the results

9.3.1 ReX_1_in.txt

- Recrystallisation path presented by the .phas-output (-1 → interface; 0 → not assigned, 1 → solid)

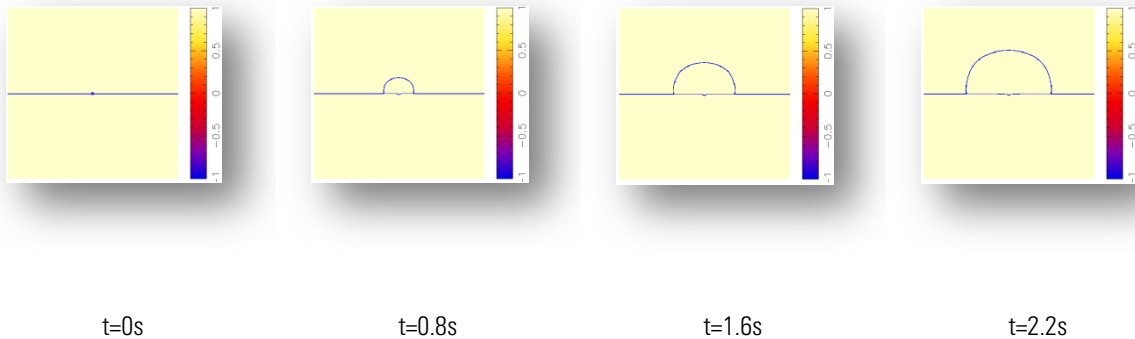


Figure 9.1. The recrystallisation sequence: Rex_1_phas.mcr. As recrystallized grains are of the same phase, they can not be distinguished in the .phas-output. Only interfaces are visible.

- Recrystallisation path presented by the .rex-output (-1 → interface; 0: new structure/recrystallized grains , 1 → not assigned, 2 → not assigned; 3 → initial structure/non-recrystallized grains)

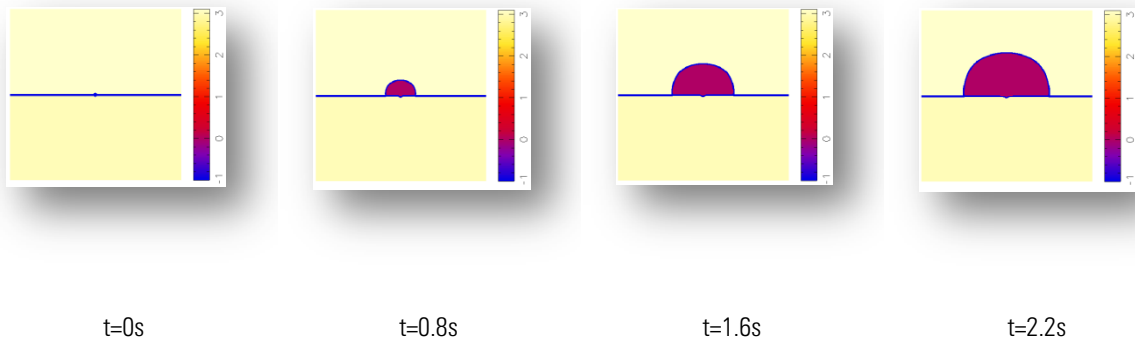


Figure 9.2. The recrystallisation sequence: Rex_1_rex.mcr. As recrystallized grains are of the same phase, they can best be distinguished in the .rex-output.



- **ReX_2_in.txt**

- Recrystallisation path presented by the .rex-output

(-1 → interface; 0: new grains, 1 → not assigned, 2 → not assigned; 3 → initial grains)

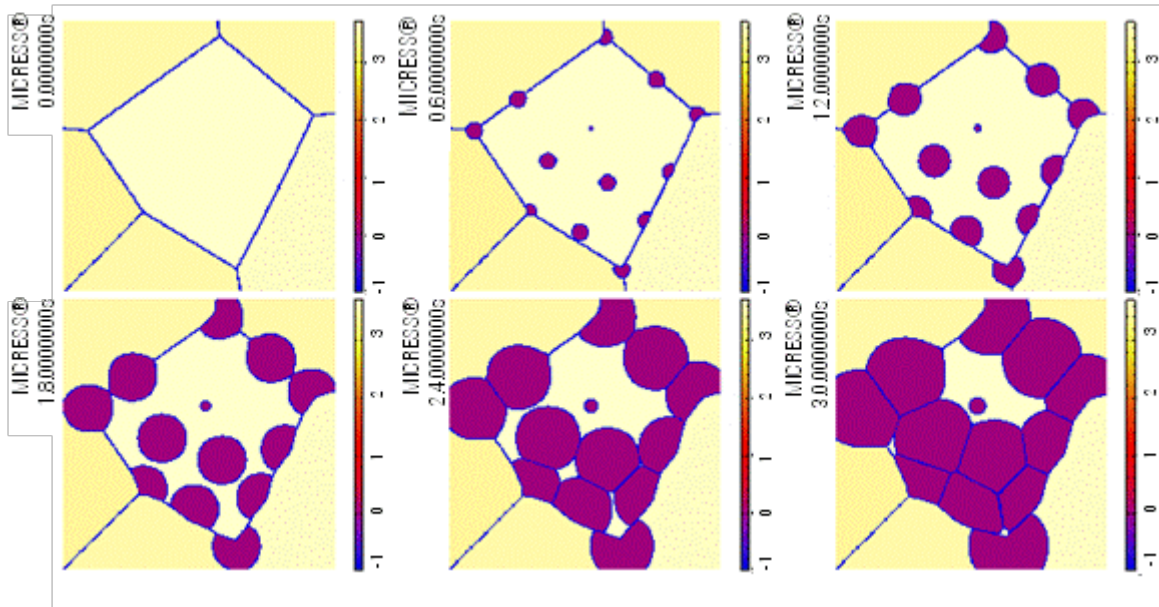


Figure 9.3: The recrystallisation sequence: Rex_2_phas.mcr

9.3.3. ReX_3_in.txt

- Recrystallisation sequence presented by the .orie-output (grain orientations)

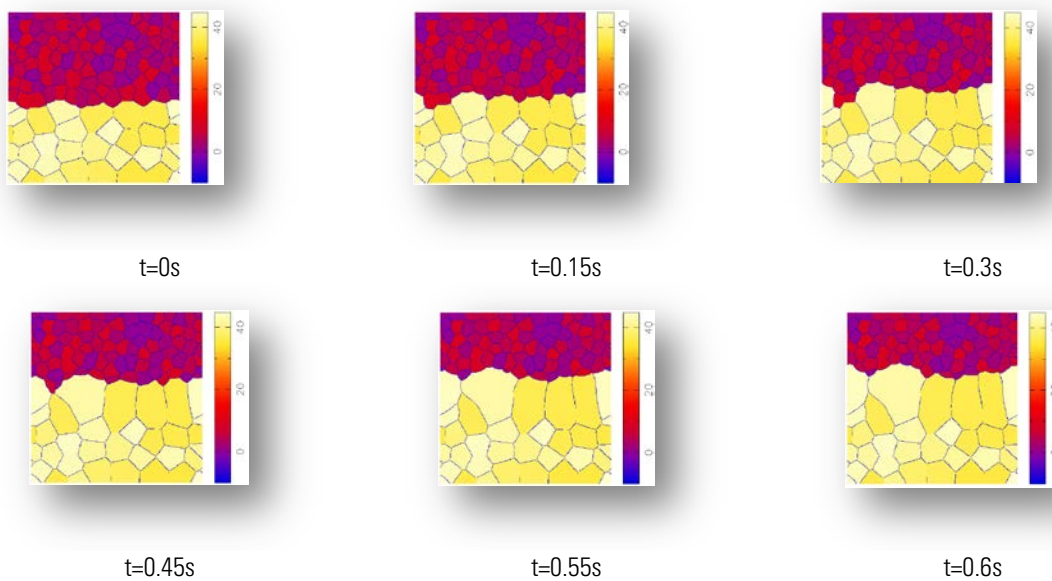


Figure 6. The recrystallisation path: Rex_3_orie.mcr. Different grains may also be distinguished by their orientation



9.3.4 ReX_4_in.txt

- Recrystallisation path presented by the .orie-output

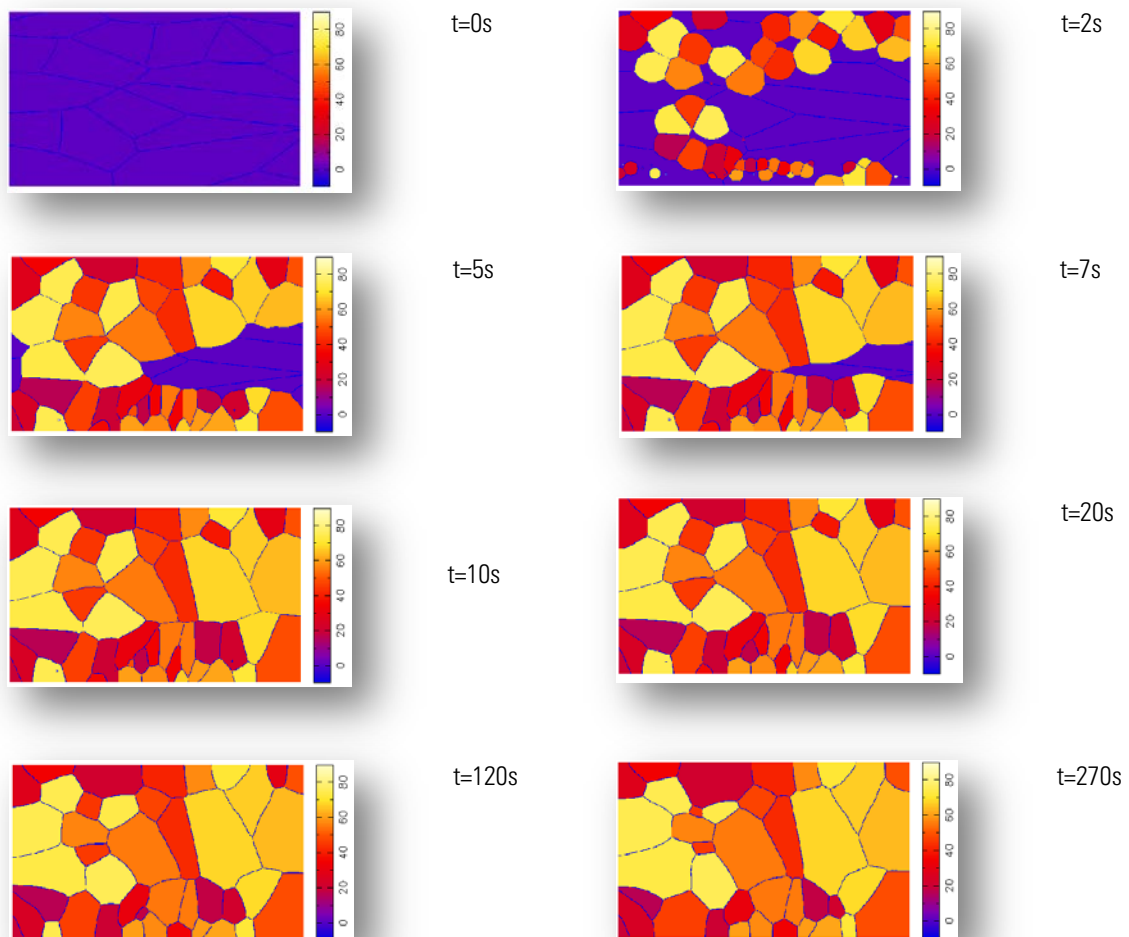


Figure 9.5. The recrystallisation path: Rex_4_orie.mcr



9.3.5 ReX_5_in.txt

- Recrystallisation path presented by the .orie-output

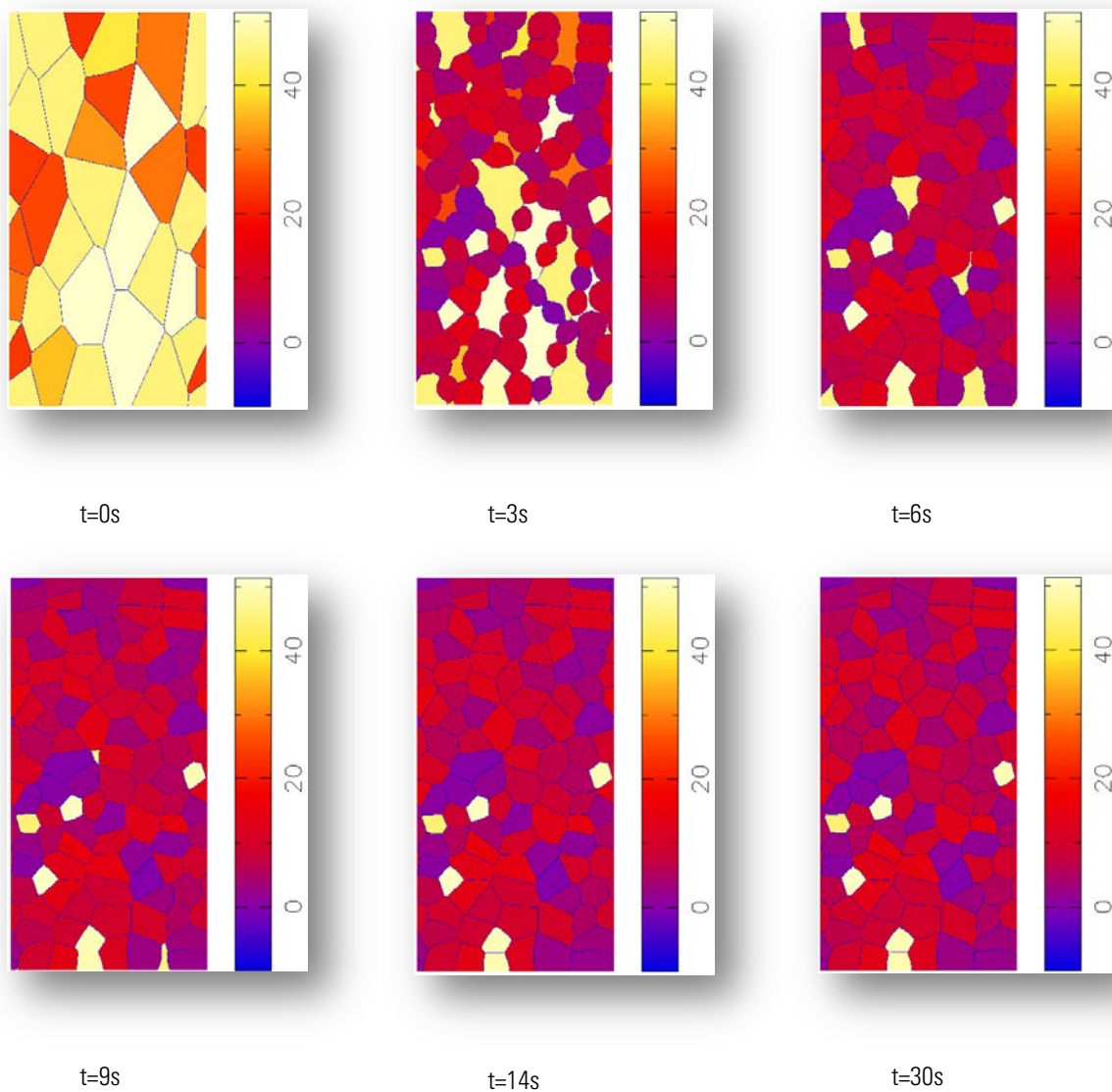


Figure 9.6. The recrystallisation path: Rex_5_orie.mcr



10 "Stress"

10.1 Description

The example "Stress_dri" is concentration-coupled and shows the simulation of Eshelby's solution.

name dri file	Stress_in.txt
alloy system	Fe-C-Mn
composition	0,103 wt% C in austenite 0,49 wt% Mn in austenite
transition	austenite to ferrite (with stress)

Table 14 Example: "Stress":- details



10.2 Simulation conditions

name dri file	Stress_in.txt
dimension	2D
grid size	200x200 cells
grid spacing	0.25 μ m
interface thickness	5.5 cells
boundary conditions BCs	
phase field BCs	East: insulation West: insulation bottom: insulation top: insulation
concentration field BCs	East: insulation West: insulation bottom: insulation top: insulation
solid phases:	2 solid phases: austenite (initial/matrix) and ferrite (growing)
grain input	<u>recrystallisation</u> : NO <u>deterministic</u> placement of one austenite grain (round $r = 1000\mu$ m position $x = 0.0$, $z = 0.0$) and one ferrite grain (round $r = 2.5\mu$ m, $x = 25.5$, $z = 24.2$) (stabilisation of the grain, no Voronoi construction) <u>further nucleation</u> : NO <u>latent heat</u> : NO <u>temperature conditions</u> : $T_0 = 1100$ K; $G = 0$ K/cm; $dT/dt = 0$ K/s <u>phase diagram input</u> : linear <u>notation of eigenstrain</u> : volume
output	<u>files</u> : interface, driving force, concentration, normal stress, von Mises stress, normal displacement <u>times</u> : -> fixed output at 0,01 s -> automatic output
special features	-> concentration coupling, stress calculation -> 1d far field diffusion approximation: NO -> thermodynamic coupling: NO -> moving frame: NO

Table 15 Example 01: Delta-Gamma: field parameters



10.3 Visualisation of the results

- The von Mises stress field presented by the .vM-output

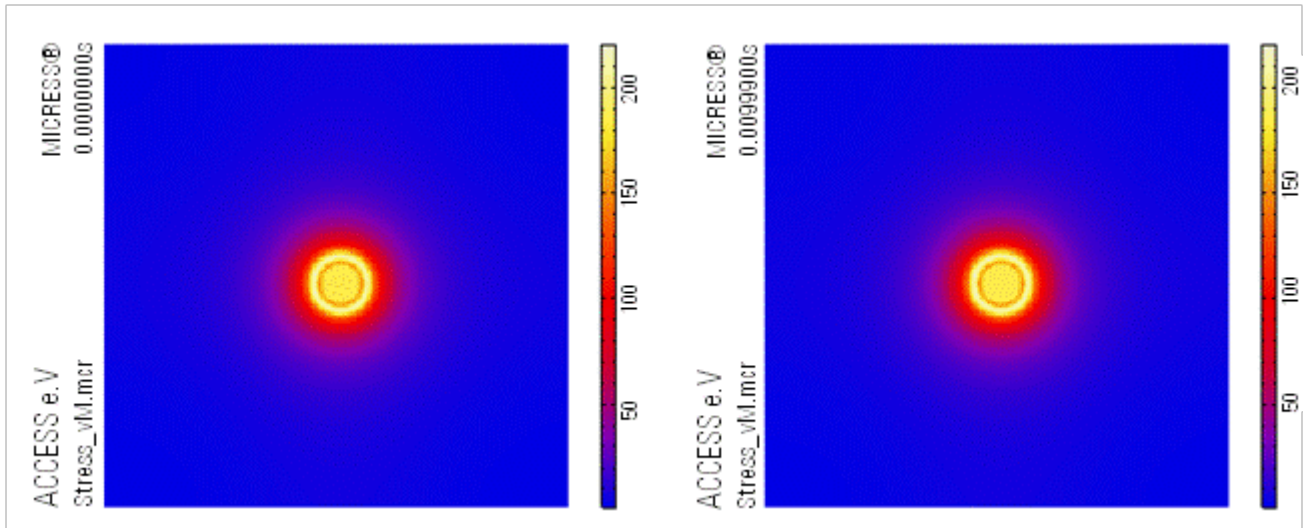
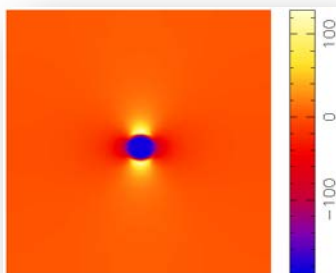
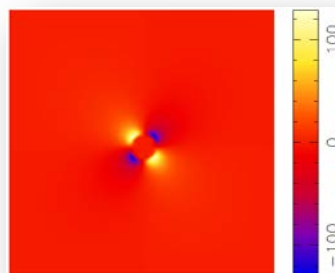


Figure 10.1. The von Mises stress field: Stress_vM.mcr

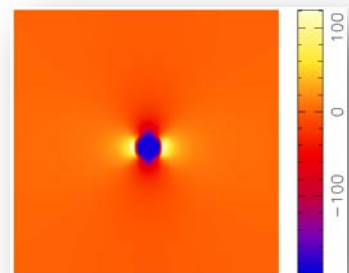
- Normal stresses in x, y and z-direction presented by the .cV-outputs



t=0s, Stress_sxxCV.mcr



t=0s, Stress_sxzCV.mcr



t=0s, Stress_szzCV.mcr

Figure 7. The normal stress distributions in different directions

11 “Basic TQ-Coupling”

11.1 Description

The two examples, “TQ_Ripening_dri” and “TQ_Eutectic_dri” illustrate the basics of the Thermo-Calc™ coupling (via its TQ interface). Here, phase transformations are simulated in an aluminium silver alloy. The first model is isothermal and shows the effect of curvature. The second one is similar and adds heat extraction and simulation of latent heat release, with growth of a primary and a secondary phase, as well as solid-solid interaction after the complete solidification.

name dri file	TQ_Ripening_in.txt TQ_Eutectic_in.txt
alloy system	Ag-Al (Seta_Bin.GES5)
composition	32 at% Ag 68 at% Al
transition	phase transformation

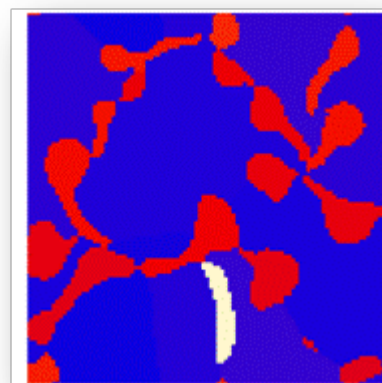


Table 16 Example: “TQ-Coupling”:- details



11.2 Simulation conditions

name dri file		TQ_Ripening_in.txt	TQ_Eutectic_in.txt
dimension		2D	
grid size (cells)		100x1x100	
grid spacing		0.1μm	
interface thickness (cells)		4	
boundary conditions BCs			
phase field BCs	East:	periodic	symmetric
	West:	periodic	symmetric
	bottom	periodic	periodic
	top:	periodic	periodic
concentration field BCs	East:	periodic	periodic
	West:	periodic	periodic
	bottom:	periodic	periodic
	top:	periodic	periodic
solid phases:		1 solid phase: FCC_A1	2 solid phases: FCC_A1, HCP_A3
grain input		<u>recrystallisation</u> : NO	
		<u>random</u> placement of grains (round); integer for randomization: 10; stabilisation of the grains; Voronoi construction	
		<u>further nucleation</u> : NO	<u>further nucleation</u> : enabled 1 type of seeds, position of the seeds: interface; maximum number of simultaneous nucleations: 25
		<u>temperature conditions</u> : T ₀ =845 K; G = 0 K/cm; dT/dt = 0 K/s	
		<u>latent heat</u> : enabled	
output		<u>files</u> : restart, grains, phases, average fraction output, interface output, driving force output, mobility output, curvature, grain-time file, concentration, concentration of the reference phase, linearization output, monitoring outputs	
		<u>times</u> : fixed output at 0.001 s logarithmic step outputs at 1.4142 s and 1 s	<u>times</u> : from 0 s to 0.02 s output every 0.005 s from 0.02 s to 0.55 s output every 0.02 s (linear step)
special features		-> concentration coupling -> NO 1d far field diffusion approximation -> thermodynamic coupling: enabled; Seta_Bin.Ges5 datafile -> NO moving frame	

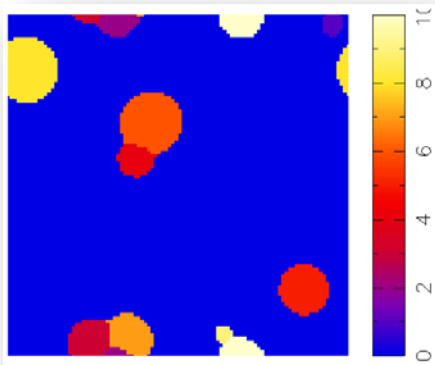
Table 17 Example: TQ_coupling: field parameters



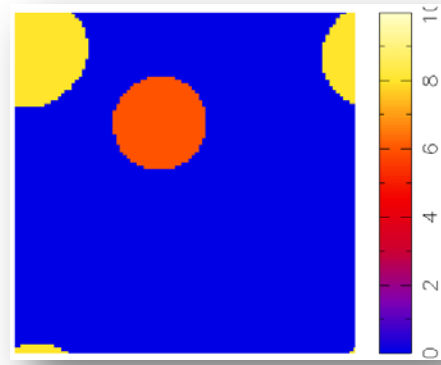
11.3 Visualisation of the results

11.3.1 “TQ_Ripening_in.txt”

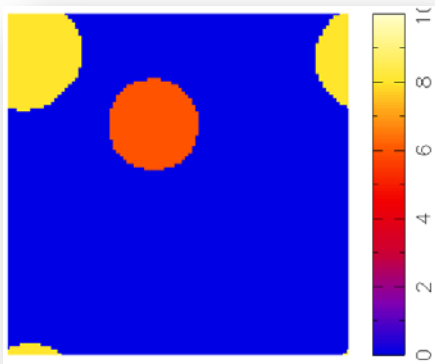
- The ripening sequence presented by the .korn-output (grain numbers)



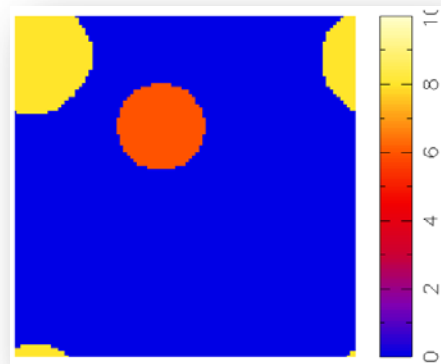
$t=0s$



$t=0.5119116s$



$t=0.7239454$



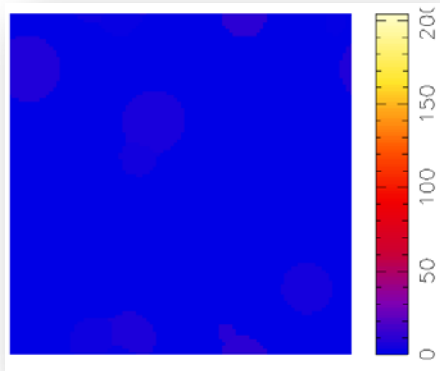
$t=1.0s$

Figure 11.1. TQ_Ripening_korn.mcr

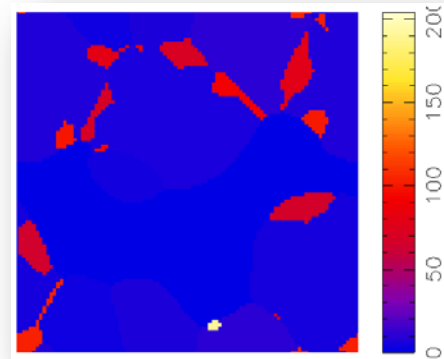


11.3.2 “TQ_Eutectic_in.txt”

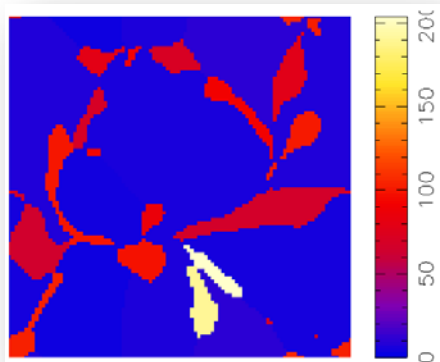
- The phase transition path presented by the .korn-output



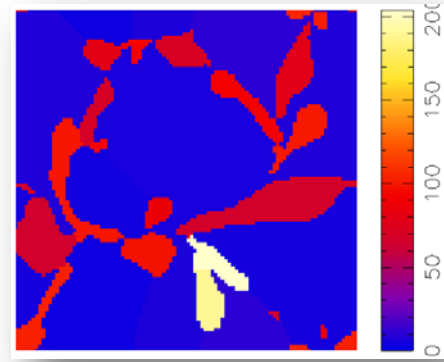
$t=0s$



$t=1s$



$t=0.34s$



$t=0.55s$

Figure 11.2. TQ_Eutectic_korn.mcr



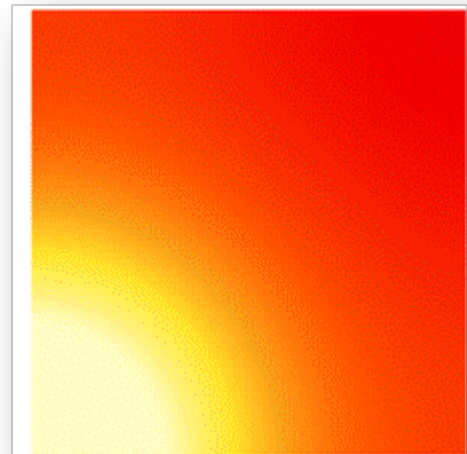
12 "Temperature"

12.1 Description

The example "Temperature_dri" illustrates the use of coupling to a temperature field for the case of a sphere of a pure substance growing into an undercooled liquid.

name dri file	Temperature_in.txt
alloy system	arbitrary model material with $T_m = 1000K$
composition	pure phase
phenomenon	Solidification of pure substance

Table 18 Example: "Temperature":- details





12.2 Simulation conditions

name dri file	Temperature_in.txt
dimension	2D
grid size	75x1x75 cells
grid spacing	1 μm
interface thickness	7 cells
boundary conditions BCs	
phase field BCs	East: insulation West: insulation bottom: insulation top: insulation
temperature field BCs	East: insulation West: insulation bottom: insulation top: insulation
solid phases:	one solid phase (a pure substance)
grain input	<u>recrystallisation</u> : NO <u>deterministic</u> placement of 1 grain (round $r = 0,0$; position $x = 0,0$, $z = 0,0$; $r=20 \mu\text{m}$); stabilisation of the grain, Voronoi construction <u>further nucleation</u> : NO <u>temperature conditions</u> : $T_{0, \text{bottom}}=999.665 \text{ K}$; $T_{0, \text{top}}=999.665 \text{ K}$
output	<u>files</u> : restart data, grain number output, phases, fraction, average fraction table, interface, driving force, mobility, curvature, velocity, grain time file, temperature, monitoring outputs <u>times</u> : -> output at 0,000001 s, 0.00001, 0.00005, 0.0001, 0.0002, 0.002 -> fixed output: time step = $1\text{E}-7$
special features	-> temperature coupling (gs) -> 1d far field diffusion approximation: NO -> thermodynamic coupling: NO -> moving frame: NO

Table 19: "Temperature" Example: simulation conditions



12.3 Visualisation of the results

- The temperature field as taken from the .temp-output

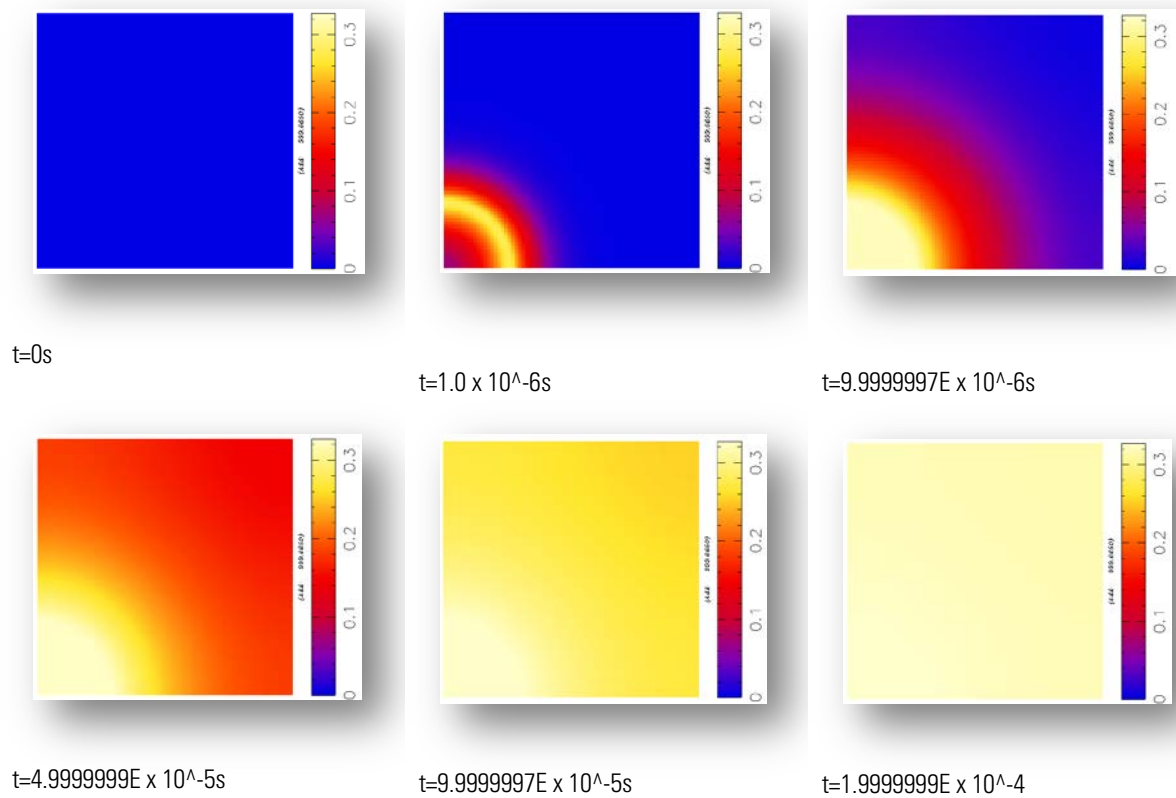


Figure 12.1. Temperature_temp.mcr



- Growth of a spherical particle as taken from the .phas-output

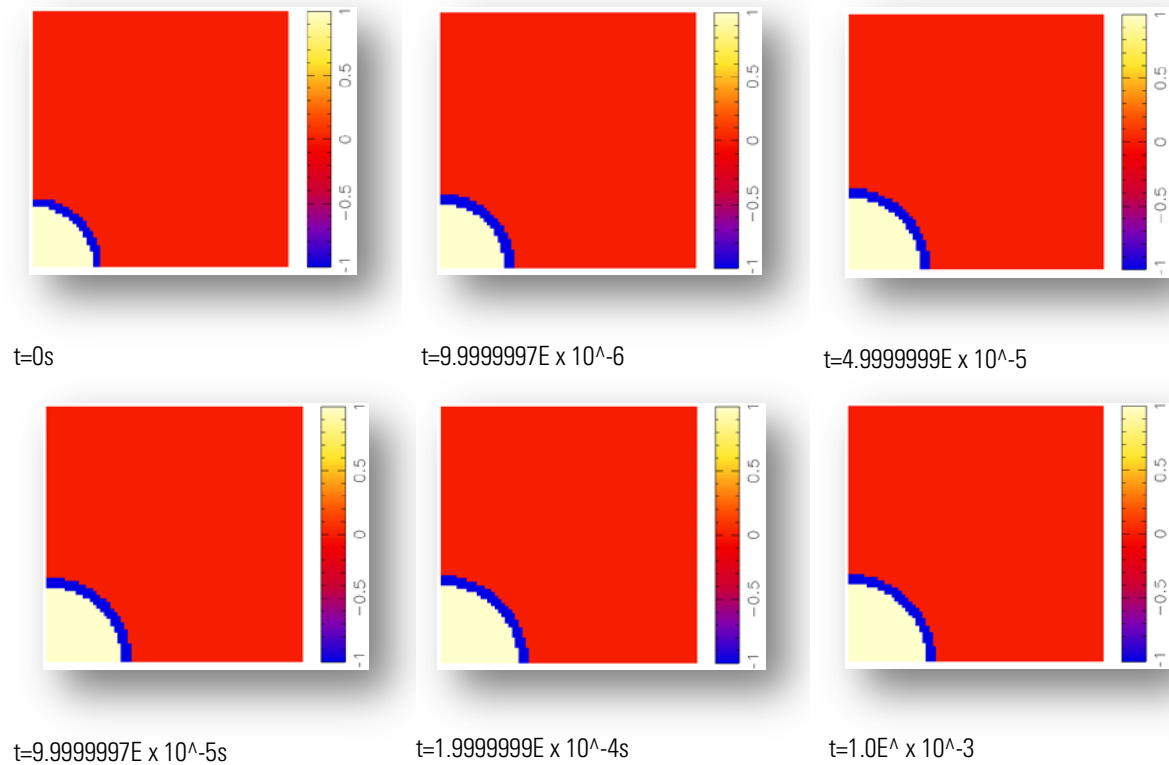


Figure 12.2. Temperature_phas.mcr



13 “Ni-based Alloy”

13.1 Description

The example “CMSX4_dri” illustrates the design of the input file for directional solidification of a complex technical alloy. The challenge here is not only the high number of elements but also the high composition level and the proximity of composition to the spinoidal decomposition region. To avoid “apparent” demixing connected with the multi-binary extrapolation scheme, the diagonal elements of the partition matrix are used instead for redistribution as invoked by the “interaction” keyword without further parameters. A further optimisation would be possible here by defining suitable ternary subsystems for more exact extrapolation.

As initial situation, 14 small grains are positioned such as to reproduce two regular grids which are connected by a grain boundary. The orientations of the cubic fcc grains has been chosen according to the typical stacking inside grains when looking at isothermal sections in directionally solidified samples. Thus, the primary dendrite arm distance λ_1 is fixed. If selection of λ_1 is the goal, a different setup of dendrites growing along a temperature gradient should be chosen.

In the course of solidification, different elements are segregated to the interdendritic liquid, leading to precipitation of γ' -phase before the end of solidification. Precipitation of this phase from the solid has not been included in this simulation setup.

Due to the high number of dissolved elements, updating thermodynamic data is very slow. For that reason, a global relinearisation scheme (keyword “global”) has been chosen as relinearisation scheme which uses only one set of linearization data for the whole interface of (e.g. a γ' particle with liquid). This is a reasonable assumption as the chemical composition of liquid around this particle is quite homogeneous and no temperature gradient is present. But for the fcc-liquid interface this is no longer true when the liquid phase splits up into smaller regions which may have different composition. Therefore the option “globalF” which is new in MICRESS® 6.2 has been used. With this relinearisation mode, fragmentation of the interface into disconnected regions is detected, and for each fragment an individual set of linearization parameters is assigned.

Note that this example further uses temperature-dependent interface mobility values as well as diffusion coefficients which are read from ascii-files during simulation. This is not so much meant for improving physical correctness but mainly for increasing performance and numerical stability while not having any substantial impact on the simulation results!



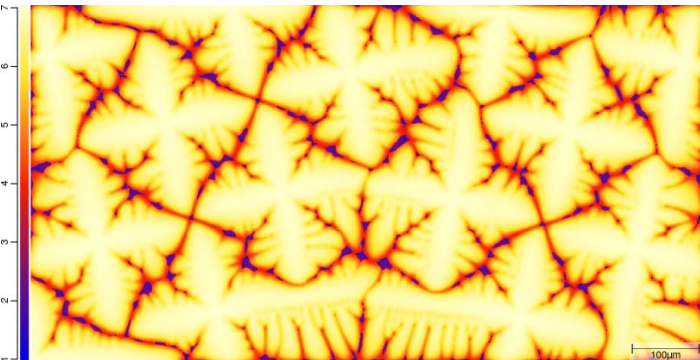
name dri file	CMSX4_dri.txt	
alloy system	CMSX4	
composition	Ni-6.5%Cr-9%Co-0.6%Mo-6%W-6.5%Ta-5.6%Al-1%Ti-3%Re-0.1%Hf	
phenomenon	Solidification and formation of interdendritic γ'	

Table 20 Example: “CMSX4” - details

13.2 Simulation conditions

name dri file	CMSX4_dri.txt
dimension	2D
grid size	1000x1x520 cells
grid spacing	1 μm
interface thickness	2.5 cells
boundary conditions BCs	
phase field BCs	East: insulation West: insulation bottom: insulation top: insulation
temperature field BCs	East: insulation West: insulation bottom: insulation top: insulation
solid phases:	FCC_A1 (γ), FCC_L12 (γ')
grain input	<u>recrystallisation</u> : NO <u>deterministic</u> placement of 14 small grains at centers of the dendrites <u>further nucleation</u> : FCC_L12 at interfaces <u>temperature conditions</u> : $T_{0, \text{bottom}}=1652$ K, constant cooling rate 0.65 K/s, no gradient



databases	<u>thermodynamic</u> : TTNi7 <u>diffusion data</u> : MOBNI1
special features	-> "interaction": diagonal mode for partition matrix -> "workspace_size": extended size of Thermo-Calc workspace -> thermodynamic coupling: YES -> relinearisation modes: "global" and "globalF"

Table 21: "Temperature" Example: simulation conditions

13.3 Visualisation of the results

Tungsten concentration for different times:

t=10s

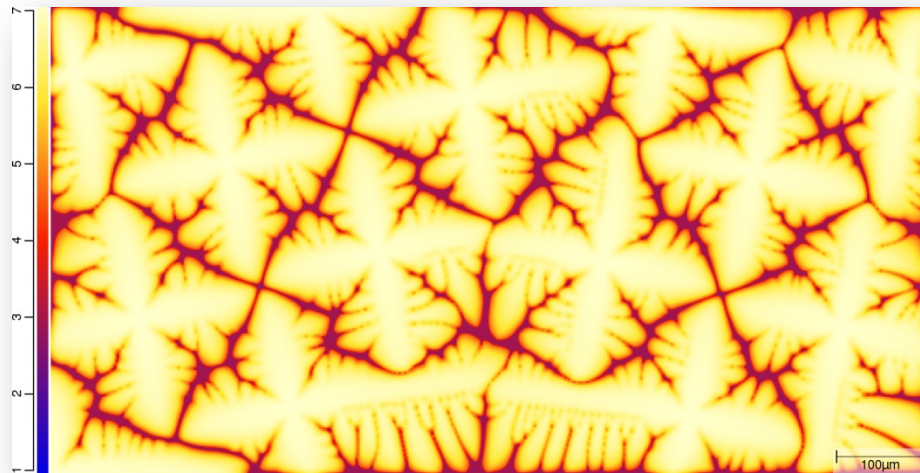


t=30s





$t=130s$



$t=400s$

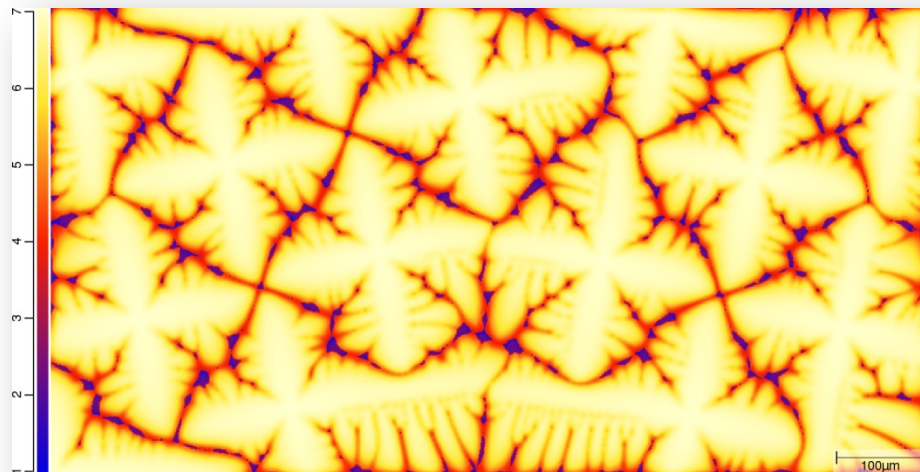


Figure 13.1. Concentration field of W after different times



14 “Dendrites”

14.1 Description

In the “Dendrite” examples dendritic solidification of an AlSi7 alloy is simulated in three dimensions. The thermodynamics for AlSi7 (liquid and fcc-Al phase) is described as a linearized phase diagram.

One objective is to demonstrate the effects of fluid flow on dendritic growth. This is done by simulating the growth of a dendrite in a forced fluid flow of 1mm/s. MICRESS® currently does not include movement of solid phases, meaning that effects of pressure or frictional forces on solid phases are neglected, so the dendrite is immobile and not transported with the fluid flow.

The melt flow affects the local concentration by advective transport. This leads to higher Si concentrations “downwind” of the solidifying dendrite leading to slower growth in direction of the melt flow. In contrast the dendrite grows faster against the flow direction where the local concentration is lowered due to the oncoming “fresh” (not Si-enriched) melt. Periodic boundary conditions for the concentration field were employed in the z-direction to keep the total Si-concentration in the simulation domain constant.

Material data for fluid flow is provided by literature: Density of liquid AlSi7 $\rho=2.7 \text{ g/cm}^3$ and the dynamic viscosity at solidification temperatures $\mu \approx 1 \cdot 10^{-3} \text{ kg/ms}$ equates to a kinematic viscosity of $\nu = \mu/\rho = 3.7 \cdot 10^{-3} \text{ cm}^2/\text{s}$.

14.2 Simulation conditions

name dri file	Dendrite_AlSi_3D.dri	Dendrite_AlSi_3D_flow.dri
dimension	3D	
grid size	100x100x100 cells	80x80x200 cells
grid spacing	2 μm	
interface	3.5 cells	



boundary conditions	Symmetric at west, south and bottom boundaries, insulation at east, north and top boundaries	Symmetric at west and south boundaries, insulation at east and north boundaries. At top and bottom periodic concentration and phase field, fixed flow of 1mm/s in z-direction.
Cooling rate	-0.3 K/s	-0.1 K/s
solid phase	Fcc-Al	
seed input	<u>One seed at origin:</u> (1,1,1) = center of the symmetric cell In lattice orientation	<u>One seed in the middle of the z-axis:</u> (1,1,200) In lattice orientation
output	<u>files:</u> fraction phase 1, concentration 1 (Si) in phase 0 (liquid) , log and fraction tables <u>times:</u> linear step 5s till 15 s	<u>files:</u> fraction phase 1, concentration 1 (Si) in phase 0 (liquid) , log and fraction tables <u>times:</u> linear step 0.5s till 2.5 s
special features	-> concentration coupling -> VTK output (viewable with ParaView) -> interface stabilisation	In addition: -> fluid flow -> piso limited by solver cycles -> analytical starting conditions for fluid flow

Table 22 Example Delta-Gamma: simulation conditions/parameters

14.3 Tweaking performance

Since 3D-simulations are computationally intensive, some measures are taken to reduce computation time, especially for fluid flow calculations. The large grid spacing of 2 μm is most helpful in this respect, since it reduces the number of simulations cells and allows larger time steps in the flow- and diffusion- parts of the simulation. To avoid deformation of the phase field at the interface on such a coarse lattice, interface stabilisation is employed by supplying an extra parameter for the interfacial energy.

The grid spacing for fluid flow is doubled by means of the "flow_coarse" option, further reducing the number of simulation cells. The orientation of the dendrite is chosen so that symmetry planes of the cubic anisotropy coincide with symmetric domain boundaries, to reduce the simulation domain.

For the forced fluid flow a fixed velocity in z-direction was set at the B- and T-boundaries. Using a pressure differential would lead to a quickly accelerating flow, especially in the beginning of the simulation when the grain is small and frictional forces are negligible. So an inflow with a fixed velocity was chosen. For the outflow conditions a fixed outflow velocity was chosen for two reasons: Fixing in- and outflow velocities leads to faster convergence of the flow solver, also it is more consistent with periodic boundary conditions for the concentration field to match the velocities of the outflow with those of the inflow.



These boundary conditions lead to a uniform velocity of the fluid at the start of the simulation when there is no solid phase. This is determined analytically using the “ana_start” option. Numerical improvement of the analytical solution is unnecessary and avoided with “pre_iter 0”. For a rough estimate of the Reynolds number the cross section can be used as a diameter $d=320\mu\text{m}$, so $\text{Re}=d\cdot v_{\text{avg}}/\nu=320\mu\text{m}\cdot 1\text{mms}^{-1}/3.7\cdot 10^{-3}\text{cm}^2\text{s}^{-1}\approx 0.86$.

So in this case “piso” and “combined” solver should perform about equally well, this example uses the piso solver. To find optimal values for time stepping tests were done starting with CFL-Limits $C_{\text{adv}}=0.3$ and $C_{\text{visc}}=0.25$ equating to a maximum time step size $\Delta t_{\text{max}}=C_{\text{visc}}\cdot(\Delta x_{\text{coarse}})^2/\nu=0.25\cdot(4\mu\text{m})^2/3.7\cdot 10^{-3}\text{cm}^2\text{s}^{-1}\approx 1\cdot 10^{-5}\text{ s}$. By observing performance when rising the maximum step size a combination of $C_{\text{adv}}=0.2$ and $\Delta t_{\text{max}}=5\cdot 10^{-4}\text{ s}$ was found to optimize performance.

To find proper convergence criteria some test runs were made with verbosity 2, observing the convergence at a simulation time when some solid has formed. In this simulation the number of inner and outer piso-cycles is set as limiting element, outer piso cycles were set to 1, inner cycles to 3 after finding that 2 inner cycles were insufficient to reach convergence.

A value of $10^{-2}/\text{s}$ was chosen to limit the continuity error. Pressure and velocity criteria were then adjusted until a sweet spot was found where the accuracy was sufficient and stricter values mainly resulted in more cycles of the linear solvers.

14.4 Results

Figure 14.1 shows the simulated dendrite (without flow) at the end of the simulation. In this stage of the simulation growth rate is mostly governed by cooling rate and dendritic ripening can be observed.

In Figure 14.2 the first 2.5 seconds of the simulation with and without flow are shown side by side. For better comparability the cooling rate in “Dendrite_AISi_3D.dri” was changed to -0.1K/s to match that of “Dendrite_AISi_3D_flow.dri”. As one can see the advective species transport shifts the concentration in the direction of the melt flow which in turn causes asymmetric growth of the dendrite.

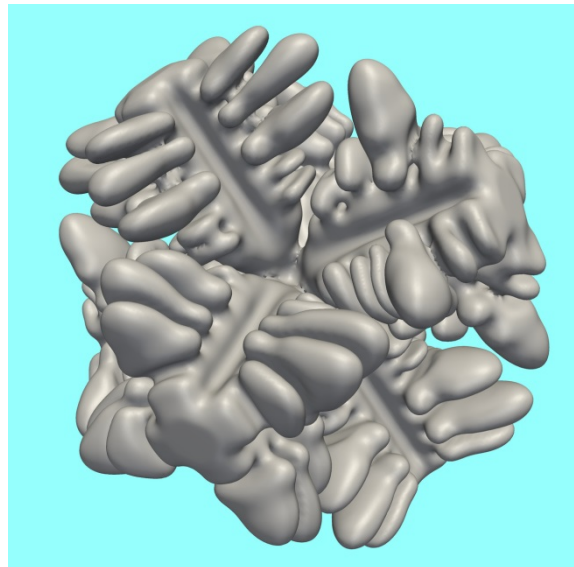


Figure 14.1: Dendrite after 15s simulation time.

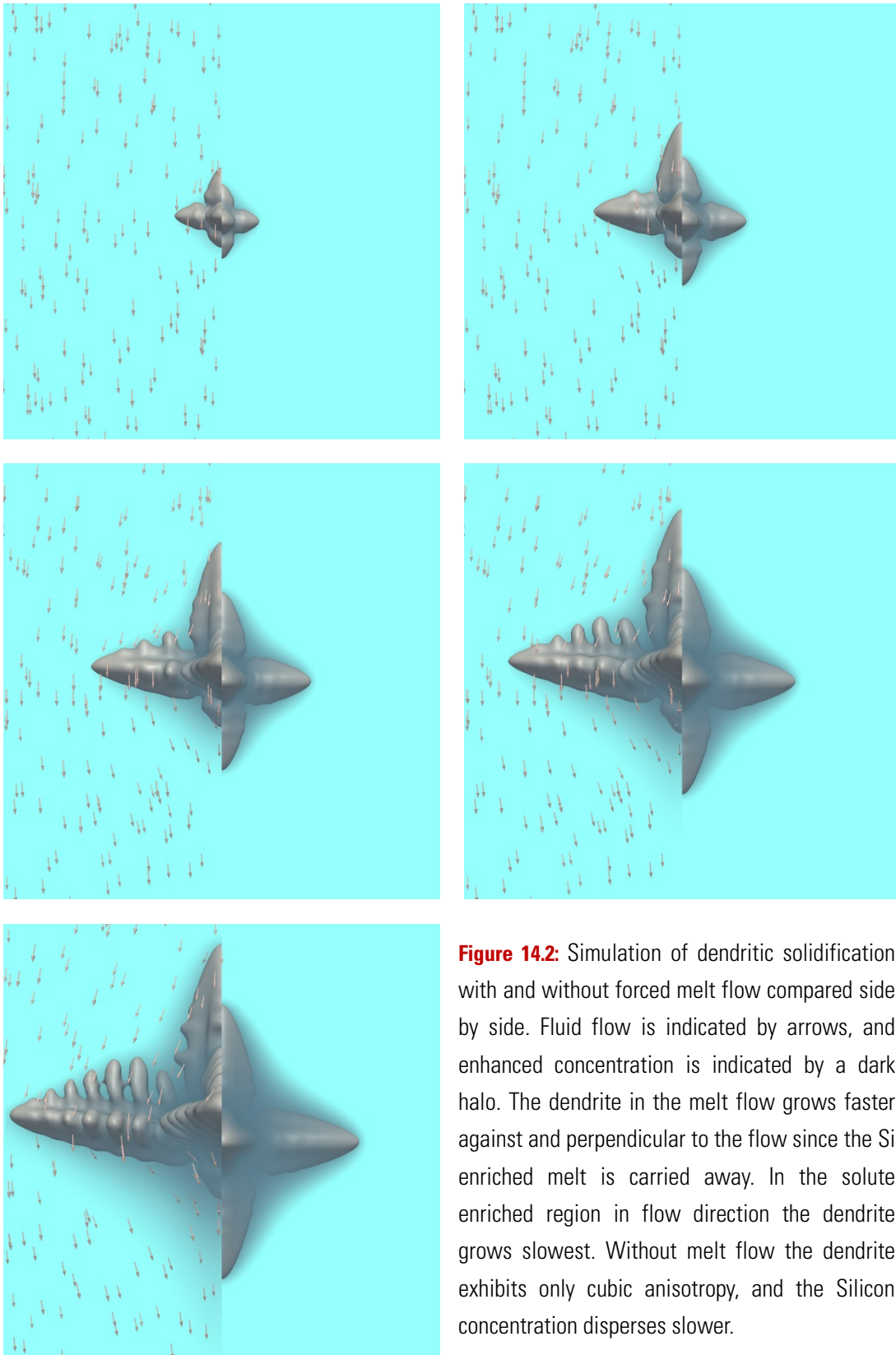


Figure 14.2: Simulation of dendritic solidification with and without forced melt flow compared side by side. Fluid flow is indicated by arrows, and enhanced concentration is indicated by a dark halo. The dendrite in the melt flow grows faster against and perpendicular to the flow since the Si enriched melt is carried away. In the solute enriched region in flow direction the dendrite grows slowest. Without melt flow the dendrite exhibits only cubic anisotropy, and the Silicon concentration disperses slower.



15 “Flow”

15.1 Description

These examples demonstrate usage of the flow solver. To simplify matters only phase field coupling is switched on and the phase field is made static by reducing the mobility. The phase field solver is only used at the beginning of the simulation, to generate a phase field profile from the sharp interface. The “Cylinder” examples demonstrate some features of the flow solver at the case of fluid flow around a static cylinder. The “Permeability” example shows the practical application of calculating the permeability for a given dendritic structure.

15.1.1 Laminar flow around a cylinder

In this case conditions were chosen so that a stationary, laminar flow around a cylinder results. The fluid flow is driven by the difference between the fixed pressures at in- and outflow. Under these conditions flow is accelerated until frictional forces compensate the driving forces. Frictionless (or gradient) boundary conditions at the top and bottom walls should be avoided here, since they would lead to unphysical situations with unending acceleration. The choice of boundary conditions has an impact on convergence and performance, for larger velocities (resulting from higher pressure gradients) the time steps must be smaller.

Since a stationary, laminar flow with $Re \ll 1$ is expected the “combined” solver is used. The time step size was determined in test runs. For the convergence criteria a limit of $10^{-2}/s$ is set for the continuity equation, matching limits for velocity and pressure are found by observing convergence in tests with higher verbosity. A value of 0.97 for pressure underrelaxation is usually a good choice with the combined solver.

15.1.2 Formation of a Karman vortex street

This is an example of a dynamically changing flow pattern resulting from a stationary geometry. This may happen when the Reynolds number is of $\sim O(10)$ or higher (depending on the geometry). In this case an inlet with a fixed velocity and an outlet with a fixed pressure are set.

For this example the “piso” solver is employed because of the higher Reynolds number. For time stepping a CFL limit (for C_{adv}) of 0.3 is used. Convergence criteria are chosen to match for a limit of $10^{-1}/s$ for the continuity equation. In this example the symmetric starting conditions result in a symmetric, nearly static state early in the



simulation until breaking of symmetry leads to dynamic changes and finally Karman vortex shedding. Notably convergence behaviour changes when the flow pattern changes, so the convergence criteria must be adjusted to work for the vortex pattern.

15.1.3 Permeability example

This is a demonstration of evaluating the permeability for a 3D structure read in from an ascii vtk file. This file contains, after a header describing the contents, a series of ones and zeroes marking cells as grain 1 (solid) or grain 0 (liquid). Such files can be produced with DP_MICRESS.

# vtk DataFile Version 3.0 vtk output ASCII DATASET STRUCTURED_POINTS DIMENSIONS 199 100 100 SPACING 1 1 1 ORIGIN 0 0 0 POINT_DATA 1990000 SCALARS solid double LOOKUP_TABLE default 0 0 0 0 0 0 0 0 ...	# vtk DataFile Version 3.0 vtk output ASCII DATASET STRUCTURED_POINTS DIMENSIONS 200 101 101 SPACING 1 1 1 ORIGIN 0 0 0 CELL_DATA 1990000 SCALARS korn float LOOKUP_TABLE default 0 0 0 0 0 0 0 0 ...
---	--

Figure 15.1: Changes to present POINT data as CELL data.

Another way is to produce legacy vtk output from ParaView (under Data -> Save Data). In this case it may be necessary to apply an image resampling filter first (with the X-, Y- and Z- cell count) to generate data on a structured grid¹. Since MICRESS[®] expects cell centred coordinates it may be necessary to edit the header as shown in Figure 15.1. After the grains are read in as grain structure the profile is adjusted to generate a smooth profile from the sharp interface (but “blocky”) grain structure. The solid fraction achieved in this way should be checked in the MICRESS[®] generated output to check if it matches the input structure with sufficient accuracy and possibly adjust the input structure (e.g. by using another threshold when marking cells as solid)².

The “steady start” option is employed to establish the flow pattern at time step 0. With this option MICRESS[®] tries to determine a large value for the time steps used to establish a steady pattern (for these steps the time limits do not apply). The number of preliminary time steps is chosen with the “pre_iter” option, it should be large enough to establish a steady fluid flow pattern. When this is the case the final time steps converge very fast, so “verbosity” should be kept at 2 for verification.

In some cases the automatic time steps may become too large to achieve convergence, especially when eddies are forming. If this is the case “freeze” the phase field as in the cylinder examples, start with small time steps and converge the flow pattern in successive runs using restarts while adjusting time steps and convergence parameters.

¹ Other filters that may prove helpful: “transform” for symmetry operations, “append datasets” to combine mirrored datasets with the original, “calculator” to generate the grain number (e.g. from phase fractions) and “pass arrays” to select only the desired output array.

² Profile adjustment can take some time for large structures, so you might want to generate a restart file with adjusted profile and start from there (with “steady_restart” or frozen phase field) when adjusting convergence parameters.



15.2 Simulation conditions

name dri file	Flow_Cylinder_Laminar_dri	Flow_Cylinder_Karman_dri	Flow_Permeability_dri
dimension	2D		3D
grid size	200x100 cells	200x75 cells	199x100x100
grid spacing	0.5 μm	2 μm	1 μm
interface	5 cells		2.5 cells
flow boundary conditions	Insulation at top and bottom, in/outflow with fixed pressure east and west	Insulation at top and bottom, Fixed velocity inflow west, fixed pressure outflow east	Symmetry at top,bottom, north and south, periodic conditions with pressure gradient for east/west
grain input	<u>One circular grain</u> : Radius 10 μm in the middle of the domain	<u>One circular grain</u> : Radius 10 μm closer to the inflow	<u>Structure from file</u> : vtk-file with cell values marking solid with 1
output	<u>files</u> : solid fraction, flow velocities and pressures		solid fraction, flow velocities
special features	-> combined solver -> fixed timestepping	-> piso solver -> cfl timestepping	-> combined solver -> steady start -> vtk output
Average v_x	1.6 $\cdot 10^3$ $\mu\text{m/s}$ (result)	1 $\cdot 10^7$ $\mu\text{m/s}$ (boundary condition)	2.8 $\cdot 10^1$ $\mu\text{m/s}$ (result)
Reynolds number	1.6 $\cdot 10^{-2}$	100	2.8 $\cdot 10^{-3}$ (100 μm domain width)
Material flow parameters	Density $\rho = 1\text{g/cm}^3$, viscosity $\nu = 1\cdot 10^{-2}\text{cm}^2/\text{s}$ (water)		$\rho = 1\text{g/cm}^3$, $\nu = 1\cdot 10^{-2}\text{cm}^2/\text{s}$

Table 23 Example Delta-Gamma: simulation conditions/parameters

15.3 Results

In figure 15.2 the flow patterns caused by a cylindrical object are compared for two different Reynolds numbers. For low Reynolds numbers a very simple stationary pattern occurs, at higher Reynolds numbers eddies will form behind the obstacle, and at even higher Reynolds numbers periodically changing patterns like a Karman vortex street may evolve after some simulation time.

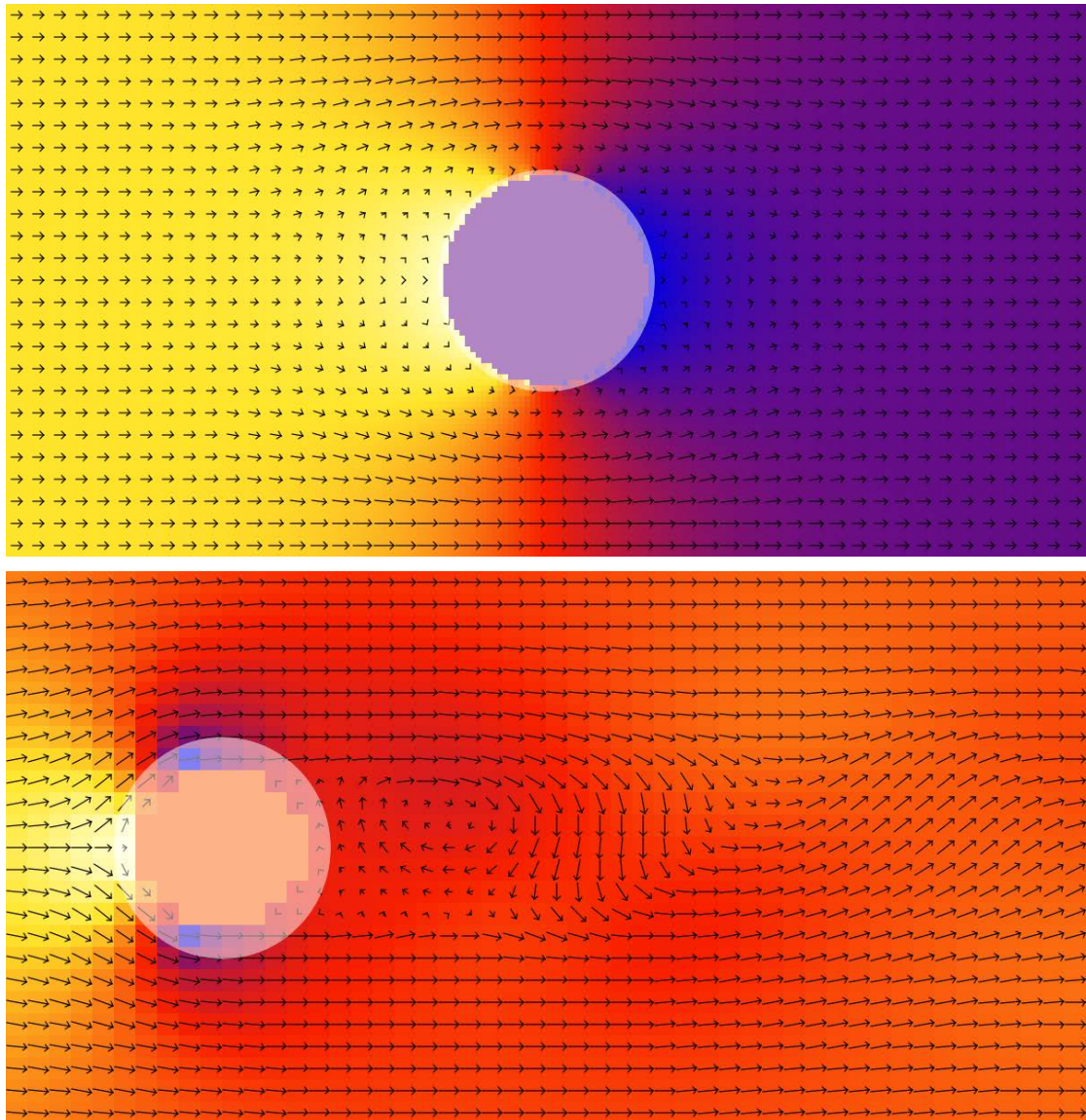


Figure 15.2: Flow around a cylinder for $Re=1.6 \cdot 10^{-2}$ (top) and $Re=100$ (bottom)

The white circle indicates the grain geometry from the driving file. In the Karman example the grid distance is quite large, so the interaction of melt flow with the phase field interface can be seen: The solid fraction has a braking effect on the fluid flow, so melt flow can pass (tangentially) through the phase field interface but is slowed down.

For the dendritic structure the simulation yields a steady velocity field with an average velocity $v_x = 2.8 \cdot 10^{-5}$ m/s. The average pressure gradient given in the input equals the pressure difference over the length in x- direction: $g = \Delta p/L = 1 \text{ Pa} / 199 \text{ }\mu\text{m} = 5 \cdot 10^3 \text{ kg/m}^2\text{s}^2$. The dynamic viscosity from the material data section for fluid flow is given by the kinematic viscosity and the density $\mu = \nu \cdot \rho = 7 \cdot 10^{-3} \text{ kg/ms}$. From these values the permeability results as:

$$k = \frac{\mu \cdot v_x}{g} = 3.9 \cdot 10^{-11} \text{ m}^2$$

The value for the liquid fraction of the simulation domain is provided in the tabulated fractions as 84%.

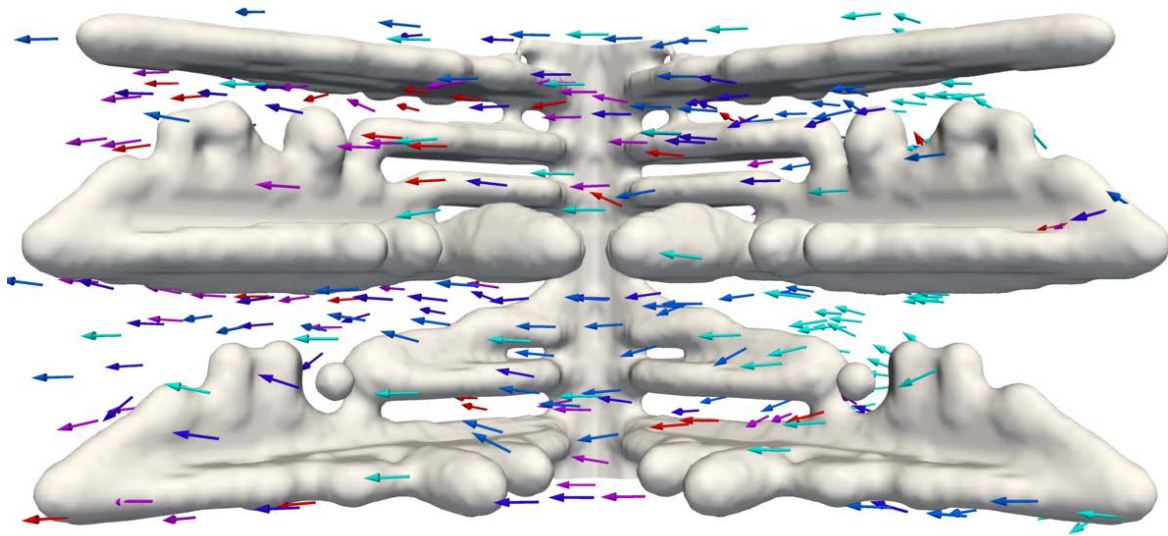


Figure 15.3: Flow through a dendritic structure